Fixed Points and Attractors of Reaction Systems*

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Abstract. We investigate the computational complexity of deciding the occurrence of many different dynamical behaviours in reaction systems, with an emphasis on biologically relevant problems (*i.e.*, existence of fixed points and fixed point attractors). We show that the decision problems of recognising these dynamical behaviours span a number of complexity classes ranging from FO-uniform AC^0 to Π_2^{P}-completeness with several intermediate problems being either NP or coNP-complete.

1 Introduction

Reaction systems (RS) are a computational model recently introduced by Ehrenfeucht and Rozenberg [5] which was inspired by chemical reactions. Interest in this model has grown due to its ability to be used to investigate practical problems while retaining a formulation clean enough to allow a theoretical investigation of its properties. One of the main research trends in RS is the study of their dynamics, like checking the complexity of the behaviours obtainable with limited resources [4] or the probability of a system to reach a halting state [3]. Other studies focused on understanding the complexity of deciding if a certain dynamical behaviour is present in a given RS or not [14,13].

The present paper follows this trend by extending the first results on complexity proved in [5,14,13], where the idea that RS can be used to evaluate Boolean formulae was introduced. In particular, we investigate the complexity of establishing if a RS admits a fixed point (NP-complete) or a fixed point attractor (NP-complete). We also study the complexity of finding if two RS share all fixed points (coNP-complete), or all fixed point attractors (Π_2^{P}-complete).

Since RS can be used to model and study biological processes [2], determining if a particular biological system exhibits a certain behaviour is an important task with potential real-life impact. The dynamics of qualitative models (*i.e.*, where

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only the presence or absence of a substance is measured), like Boolean networks, has always been important in the modelling of biological systems. For example, attractors can represent cellular types or cellular states (*cf.*, proliferation or differentiation) [16] and determining the presence of fixed points and cycles is essential when modelling gene regulatory networks [8,1]. Furthermore, in [9] the importance of studying robustness in complex biological systems is highlighted. The identification of attractors is a necessary first step in this direction.

The paper is structured as follows. Section 2 provides the basic notions on RS and a short comparison with related models. Section 3 gives a description in logical terms of the problems we investigate. The decision problems regarding fixed points are collected in Section 4 and the ones regarding fixed point attractors in Section 5. A summary of the results and of possible future developments is given in Section 6.

2 Basic Notions

We recall the definitions of reaction, reaction system, and the associated notation from [5].

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 subsets of S. The set R_a is called the set of* reactants*, I_a the set of* inhibitors*, and P_a is the set of* products*. Denote by $\mathrm{rac}(S)$ the set of all reactions over S.*

Definition 2. *A* reaction system *$\mathcal{A}$ is a pair (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* $\mathrm{res}_a \colon 2^S \to 2^S$ of a, where 2^S denotes the power set of S, is defined as

$$\mathrm{res}_a(T) = \begin{cases} P_a & \text{if } a \text{ is enabled in } T \\ \varnothing & \text{otherwise.} \end{cases}$$

The definition of res_a naturally extends to sets of reactions. Indeed, 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.*, it is the result function of the whole set of reactions.

Example 1 (XOR gate). Consider the RS $\mathcal{A} = (\{1_0, 1_1, 1_{\mathrm{out}}\}, A)$, where the entities represent the first two inputs and the output when they assume value 1, respectively. The set A contains $(\{1_0\}, \{1_1\}, \{1_{\mathrm{out}}\})$ and $(\{1_1\}, \{1_0\}, \{1_{\mathrm{out}}\})$. The system, starting from a state that is a subset of $\{1_0, 1_1\}$ encoding the bits set to 1 in the input, produces 1_{out} in one step iff the XOR gate on the same input produces 1.

In the sequel, we are interested in the dynamics of RS, *i.e.*, the study of the successive states of the system under the action of the result function $\mathrm{res}_{\mathcal{A}}$

starting from some initial set of entities. Given a set $T \subseteq S$, the sequence of states visited by the system is $(T, \mathrm{res}_{\mathcal{A}}(T), \mathrm{res}_{\mathcal{A}}^2(T), \ldots)$ (*i.e.*, for every $t \in \mathbb{N}$, the t-th element of the sequence is $\mathrm{res}_{\mathcal{A}}^t(T)$). Since S is finite any sequence of visited states is ultimately periodic, *i.e.*, for any $T \subseteq S$, there exist $h, p \in \mathbb{N}$ such that for all $t \in \mathbb{N}$ we have $\mathrm{res}_{\mathcal{A}}^{h+pt}(T) = \mathrm{res}_{\mathcal{A}}^{h+t}(T)$; here h is the *length of the transient*. A state $T \subseteq S$ is part of a *cycle* if the sequence of states starting from T is ultimately periodic with a transient of length 0; in this case, the least p satisfying the previous equation is called the *period* of the cycle. A *fixed point* T is a cycle with period 1 (*i.e.*, $\mathrm{res}_{\mathcal{A}}(T) = T$). An *attractor* of an RS $\mathcal{A}$ is a cycle $T_1, \ldots, T_p$ for which there exists a state U not belonging to the cycle such that $\mathrm{res}_{\mathcal{A}}(U) = T_i$ for some $1 \leq i \leq p$. A *fixed point attractor* is a fixed point that is also an attractor. Given a RS $\mathcal{A}$, we say that a state T is a fixed point (resp., attractor) for $\mathcal{A}$ if it is a fixed point (resp., attractor) for $\mathrm{res}_{\mathcal{A}}$.

2.1 Related Models

Other bio-inspired models having features in common with RS are membrane systems, Boolean networks, and chemical reaction networks.

Membrane systems [11] also provide an idealisation of chemical reactions in the context of a cell. The main difference between RS and membrane systems is the presence of multiplicity, that is, the state of the membrane system is a multiset and not a set, and the rewriting rules consume the substances that they use. Furthermore, the main characteristic of membrane systems is the presence of membranes that partition the system into multiple regions with limited communications. The idea of linking membrane systems and RS is not new and has already been explored [12].

Synchronous Boolean networks [7,15] can be viewed as a generalisation of RS. Indeed, they can be used to simulate RS by associating an entity to each node of the network; the value of a node denotes the absence or presence of an entity in the current state of the simulated RS, that is, the state of the Boolean network is the characteristic vector of the state of the RS. The update function of a node can be written as a Boolean formula in disjunctive normal form that holds iff the entity denoted by the node is generated by some reaction of the RS. The resulting Boolean network has a description of polynomial length with respect to the description of the RS. The converse simulation, while possible, might require an exponential number of reactions, depending on the encoding of the Boolean network.

Chemical reaction networks (CRN) are a model in which a set of entities (called *signals* in CRN) is modified by means of chemical reactions described by reactants, products, and catalysts [18]. Reactants are consumed to generate the products when both they and the catalysts are present in the current state of the system. The operations of CRN can be implemented in multiple ways, for example by means of logical circuits or DNA strand displacement systems. The main differences between CRN and RS are that the state used by the former is a multiset (*i.e.*, the multiplicity is considered) and there are no inhibitors in the reactions.

3 Logical Description

This section provides a tool that will be used in many proofs of the paper. It consists of a logical description of RS and formulae related to their dynamics. This description (or a slight adaptation) will be sufficient for proving membership in many complexity classes. For the background notions of logic and descriptive complexity we refer the reader to Neil Immerman's classical book [6].

In the sequel, we will study several classes of problems over RS, and each of them can be characterised by a logical formula. A RS $\mathcal{A} = (S, A)$ with background set $S \subseteq \{0, \ldots, n-1\}$ and $|A| \leq n$ can be described by the vocabulary $(\mathsf{S}, \mathsf{R}_\mathcal{A}, \mathsf{I}_\mathcal{A}, \mathsf{P}_\mathcal{A})$, where S is a unary relation symbol and $\mathsf{R}_\mathcal{A}$, $\mathsf{I}_\mathcal{A}$, and $\mathsf{P}_\mathcal{A}$ are binary relation symbols. The intended meaning of the symbols is the following: the set of entities is $S = \{i : \mathsf{S}(i)\}$ and each reaction $a_j = (R_j, I_j, P_j) \in A$ is described by the sets $R_j = \{i \in S : \mathsf{R}_\mathcal{A}(i,j)\}$, $I_j = \{i \in S : \mathsf{I}_\mathcal{A}(i,j)\}$, and $P_j = \{i \in S : \mathsf{P}_\mathcal{A}(i,j)\}$.

We will also need some additional vocabularies: $(\mathsf{S}, \mathsf{R}_\mathcal{A}, \mathsf{I}_\mathcal{A}, \mathsf{P}_\mathcal{A}, \mathsf{T})$, where T is a unary relation representing a subset of S, $(\mathsf{S}, \mathsf{R}_\mathcal{A}, \mathsf{I}_\mathcal{A}, \mathsf{P}_\mathcal{A}, \mathsf{T}_1, \mathsf{T}_2)$ with two additional unary relations representing sets, and $(\mathsf{S}, \mathsf{R}_\mathcal{A}, \mathsf{I}_\mathcal{A}, \mathsf{P}_\mathcal{A}, \mathsf{R}_\mathcal{B}, \mathsf{I}_\mathcal{B}, \mathsf{P}_\mathcal{B})$ denoting two RS over the same background set.

The following formulae describe basic properties of $\mathcal{A}$. The first is true if a reaction a_j is enabled in T:

$$\textsc{en}_\mathcal{A}(j, T) \equiv \forall i(\mathsf{S}(i) \Rightarrow (\mathsf{R}_\mathcal{A}(i,j) \Rightarrow T(j)) \wedge (\mathsf{I}_\mathcal{A}(i,j) \Rightarrow \neg T(j)))$$

the latter is verified if $\text{res}_\mathcal{A}(T_1) = T_2$ for $T_1, T_2 \subseteq S$:

$$\textsc{res}_\mathcal{A}(T_1, T_2) \equiv \forall i(\mathsf{S}(i) \Rightarrow (T_2(i) \Leftrightarrow \exists j(\textsc{en}_\mathcal{A}(j, T_1) \wedge \mathsf{P}_\mathcal{A}(i,j))).$$

Since $\textsc{en}_\mathcal{A}$ and $\textsc{res}_\mathcal{A}$ are both first-order (FO) formulae, the following is immediately proved.

Theorem 1. *Given a RS $\mathcal{A} = (S, A)$ and two sets $T_1, T_2 \subseteq S$, deciding whether $\text{res}_\mathcal{A}(T_1) = T_2$ is in FO (which is equivalent to FO-uniform AC^0 [6]).* □

FO logic will quickly prove insufficient for our purposes; therefore we will formulate some problems using stronger logics: existential second order logic $\mathsf{SO}\exists$ characterising NP (Fagin's theorem); universally quantified second order logic $\mathsf{SO}\forall$ giving coNP; second order logic with one alternation of universal and existential quantifiers ($\mathsf{SO}\forall\exists$, giving Π_2^P). As an abbreviation, we define the bounded second order quantifiers $(\forall X \subseteq Y)\,\varphi$ and $(\exists X \subseteq Y)\,\varphi$ as a shorthand for $\forall X(\forall i(X(i) \Rightarrow Y(i)) \Rightarrow \varphi)$ and $\exists X(\forall i(X(i) \Rightarrow Y(i)) \wedge \varphi)$. We say that a formula is $\mathsf{SO}\exists$, $\mathsf{SO}\forall$, or $\mathsf{SO}\forall\exists$ if it is logically equivalent to a formula in the required prenex normal form.

4 Fixed Points

We investigate the complexity of determining if a given state is a fixed point for an RS, if an RS admits fixed points, and if two RS share at least one or all fixed points. First, we are interested in determining if the first-order formula $\text{FIX}_{\mathcal{A}}(T) \equiv \text{RES}_{\mathcal{A}}(T, T)$ holds for a given state T. Substituting $T_2 = T_1$ in Theorem 1, we get the following corollary:

Corollary 1. *Given a RS $\mathcal{A} = (S, A)$ and a state $T \subseteq S$, deciding whether T is a fixed point of* $\text{res}_{\mathcal{A}}$ *is in* FO. □

As usual, CNF (resp., DNF) means conjunctive (resp., disjunctive) normal form. Given a formula φ in CNF, we denote by $\text{neg}(\varphi)$ (resp., $\text{pos}(\varphi)$) the set of variables that occur negated (resp., non-negated) in φ. The notation $t \vDash \varphi$ means that φ is satisfied by the assignment t.

While it is easy to decide if a point is fixed, determining if a RS admits a fixed point is a vastly more difficult task as proved by the following theorem.

Theorem 2. *Given a RS $\mathcal{A} = (S, A)$, it is* NP*-complete to decide if $\mathcal{A}$ has a fixed point.*

Proof. The problem is in NP, since $(\exists T \subseteq \mathsf{S})\, \text{FIX}_{\mathcal{A}}(T)$ is a $\mathsf{SO}\exists$ formula. In order to show NP-hardness, we reduce SAT [10] to this problem. Given a Boolean formula $\varphi \equiv \varphi_1 \wedge \cdots \wedge \varphi_m$ in CNF over the variables $V = \{x_1, \ldots, x_n\}$, construct a RS $\mathcal{A} = (S, A)$ with $S = V \cup \{\spadesuit, \clubsuit\}$ and the following reactions:

$$(\text{neg}(\varphi_j), \text{pos}(\varphi_j) \cup \{\clubsuit, \spadesuit\}, \{\spadesuit\}) \qquad \text{for } 1 \leq j \leq m \qquad (1)$$
$$(\{x_i\}, \varnothing, \{x_i\}) \qquad \text{for } 1 \leq i \leq n \qquad (2)$$
$$(\{\spadesuit\}, \varnothing, \{\clubsuit\}) \qquad (3)$$
$$(\{\clubsuit\}, \{\spadesuit\}, \{\spadesuit\}). \qquad (4)$$

Given a state $T \subseteq S$, let $X = T \cap V$. The set X encodes an assignment of φ in which the variables having true value are those in X. Reactions of type (1) generate $\spadesuit$ when there exists a clause φ_j not satisfied by X (hence φ itself is not satisfied). Reactions of type (2) preserve the current assignment in the next state. Finally, reactions (3) and (4) rewrite $\spadesuit$ into $\clubsuit$ and $\clubsuit$ into $\spadesuit$ (if $\spadesuit$ is missing). Hence, the RS behaves as follows:

$$\text{res}_{\mathcal{A}}(T) = \begin{cases} (T \cap V) = T & \text{if } T \subseteq V \wedge T \vDash \varphi \\ (T \cap V) \cup \{\spadesuit\} & \text{if } (T \subseteq V \wedge T \nvDash \varphi) \vee (\clubsuit \in T \wedge \spadesuit \notin T) \\ (T \cap V) \cup \{\clubsuit\} & \text{if } \spadesuit \in T \end{cases}$$

i.e., there exists a fixed point if and only if φ is satisfiable. The mapping $\varphi \mapsto \mathcal{A}$ is computable in polynomial time, hence deciding the existence of fixed points is NP-hard. □

A direct consequence of the theorem above is that determining if there exists a state that is a fixed point in common between two RS remains NP-complete.

Corollary 2. *Given two RS $\mathcal{A}$ and $\mathcal{B}$ over the same background set S, deciding if $\mathcal{A}$ and $\mathcal{B}$ have a common fixed point is* NP*-complete.*

Proof. The problem lies in NP, since $(\exists T \subseteq \mathsf{S})(\text{FIX}_{\mathcal{A}}(T) \wedge \text{FIX}_{\mathcal{B}}(T))$ is a $\mathsf{SO}\exists$ formula. By letting $\mathcal{A} = \mathcal{B}$, NP-hardness follows from Theorem 2. □

Differently from above, determining if two reaction systems have all fixed points in common is in coNP, instead of NP. This is expected since the description of the problem involves universal instead of existential quantification.

Theorem 3. *Given two RS $\mathcal{A} = (S, A)$ and $\mathcal{B} = (S, B)$, it is coNP-complete to decide whether $\mathcal{A}$ and $\mathcal{B}$ share all their fixed points.*

Proof. The problem lies in coNP, since $(\forall T \subseteq \mathsf{S})(\text{FIX}_{\mathcal{A}}(T) \Leftrightarrow \text{FIX}_{\mathcal{B}}(T))$ is a $\mathsf{SO}\forall$ formula. In order to show coNP-hardness, we reduce $\mathsf{TAUTOLOGY}$ (also known as $\mathsf{VALIDITY}$ [10]) to this problem. Given a Boolean formula $\varphi = \varphi_1 \vee \cdots \vee \varphi_m$ in DNF over the variables $V = \{x_1, \ldots, x_n\}$, build the RS $\mathcal{A}$ consisting of the background set $S = V \cup \{\heartsuit\}$ and the following reactions:

$$(\text{pos}(\varphi_j) \cup \{\heartsuit\}, \text{neg}(\varphi_j), \{\heartsuit\}) \qquad \text{for } 1 \leq j \leq m \tag{5}$$

$$(\{x_i, \heartsuit\}, \varnothing, \{x_i\}) \qquad \text{for } 1 \leq i \leq n. \tag{6}$$

Let T be a state of $\mathcal{A}$ and $X = T \cap V$. When $\heartsuit \in T$, each reaction of type (5) evaluates a term φ_j under the assignment encoded by X, producing $\heartsuit$ when $X \vDash \varphi_j$ (hence $X \vDash \varphi$). Reactions of type (6) preserve the state when $\heartsuit \in T$. Thus the RS behaves as follows:

$$\text{res}_{\mathcal{A}}(T) = \begin{cases} T & \text{if } T \cap V \vDash \varphi \text{ and } \heartsuit \in T \\ T - \{\heartsuit\} & \text{if } T \cap V \nvDash \varphi \text{ and } \heartsuit \in T \\ \varnothing & \text{if } \heartsuit \notin T. \end{cases}$$

The fixed points of $\mathcal{A}$ are $\varnothing$ and all states of the form $X \cup \{\heartsuit\}$ with $X \subseteq V$ and $X \vDash \varphi$. Now let $\mathcal{B}$ be defined by the following reactions:

$$(\{x_i, \heartsuit\}, \varnothing, \{x_i\}) \qquad \text{for } 1 \leq i \leq n$$

$$(\{\heartsuit\}, \varnothing, \{\heartsuit\}).$$

They preserve the current state T if $\heartsuit \in T$ and yield $\varnothing$ otherwise. Hence, the fixed points of $\mathcal{B}$ are $\varnothing$ and all states of the form $X \cup \{\heartsuit\}$ with $X \subseteq V$.

By construction, the two RS $\mathcal{A}$ and $\mathcal{B}$ share all fixed points exactly when all assignments satisfy φ. Since the mapping $\varphi \mapsto (\mathcal{A}, \mathcal{B})$ is computable in polynomial time, deciding the former property is coNP-hard. □

5 Fixed Point Attractors

In this section we investigate the same problems of Section 4 reformulated for fixed point attractors.

The fact that a set T is a fixed point attractor can be expressed by the following formula: $\text{ATT}_{\mathcal{A}}(T) \equiv (\exists U \subseteq \mathsf{S})(\text{FIX}_{\mathcal{A}}(T) \wedge \text{RES}_{\mathcal{A}}(U, T) \wedge \neg\text{RES}_{\mathcal{A}}(T, U))$.

Theorem 4. *Given a RS $\mathcal{A} = (S, A)$ and a state $T \subseteq S$, it is* NP*-complete to decide whether T is a fixed point attractor.*

Proof. Since $\text{ATT}_{\mathcal{A}}(T)$ is a $\mathsf{SO}\exists$ formula, the problem lies in NP. We reduce SAT to this problem. Given a formula $\varphi = \varphi_1 \wedge \cdots \wedge \varphi_m$ in CNF over the set of variables $V = \{x_1, \ldots, x_m\}$, let $C = \{\varphi_1, \ldots, \varphi_n\}$ and let $\mathcal{A}$ be the RS having the background set $S = V \cup C \cup \{\spadesuit, \clubsuit\}$ and the following reactions:

$$(\{x\}, C \cup \{\spadesuit, \clubsuit\}, \{\varphi_j\}) \qquad \text{for } 1 \le j \le m \text{ and } x \in \text{pos}(\varphi_j) \tag{7}$$
$$(\varnothing, C \cup \{x, \spadesuit, \clubsuit\}, \{\varphi_j\}) \qquad \text{for } 1 \le j \le m \text{ and } x \in \text{neg}(\varphi_j) \tag{8}$$
$$(C, S - C, C) \tag{9}$$
$$(\text{neg}(\varphi_j), \text{pos}(\varphi_j) \cup C \cup \{\spadesuit, \clubsuit\}, \{\spadesuit\}) \qquad \text{for } 1 \le j \le m \tag{10}$$
$$(\{\spadesuit\}, \varnothing, \{\clubsuit\}) \tag{11}$$
$$(\{\clubsuit\}, \{\spadesuit\}, \{\spadesuit\}). \tag{12}$$

If the state of $\mathcal{A}$ is $X \subseteq V$, the reactions of kinds (7) and (8) produce the subset of C corresponding to the clauses of φ satisfied by X. If all clauses are generated (*i.e.*, $X \vDash \varphi$), they are preserved by reaction (9). On the other hand, if at least one clause is not satisfied by X, one or more reactions of type (10) are enabled and produce $\spadesuit$. As in the proof of Theorem 2, reactions (11) and (12) generate a cycle between the states $\{\spadesuit\}$ and $\{\clubsuit\}$. The result function of $\mathcal{A}$ is then

$$\text{res}_{\mathcal{A}}(T) = \begin{cases} C & \text{if } T = C \text{ or if } T \subseteq V \text{ and } T \vDash \varphi \\ D \cup \{\spadesuit\} & \text{if } T \subseteq V,\ D \subsetneq C \text{ and } T \text{ satisfies the clauses in } D \\ & \quad \text{but not the clauses in } C - D \\ \{\clubsuit\} & \text{if } \spadesuit \in T \\ \{\spadesuit\} & \text{if } \clubsuit \in T \text{ and } \spadesuit \notin T \\ \varnothing & \text{otherwise.} \end{cases}$$

Notice that $\mathcal{A}$ has exactly one fixed point, the state C, which is reachable from another state T (*i.e.*, C is an attractor) iff $T \subseteq V$ and $T \vDash \varphi$, *i.e.*, iff φ is satisfiable. Since the mapping $\varphi \mapsto \mathcal{A}$ can be computed in polynomial time, the NP-hardness of the problem follows. □

As immediate corollaries, finding if a fixed point attractor exists or if it exists as a shared fixed point between two RS, remain NP-complete.

Corollary 3. *Given a RS $\mathcal{A} = (S, A)$, deciding if $\mathcal{A}$ has a fixed point attractor is an* NP*-complete problem.*

Proof. The problem is in NP, since $(\exists T \subseteq \mathsf{S})\ \text{ATT}_{\mathcal{A}}(T)$ is a $\mathsf{SO}\exists$ formula. Its NP-hardness follows from the construction in the proof of Theorem 4, where for any Boolean formula φ in CNF, the RS $\mathcal{A}$ has exactly one fixed point, which is an attractor iff φ is satisfiable. □

Corollary 4. *Given two RS $\mathcal{A}$ and $\mathcal{B}$ with the same background set S, it is* NP*-complete to decide whether $\mathcal{A}$ and $\mathcal{B}$ have a common fixed point attractor.*

Proof. The problem lies in NP since $(\exists T \subseteq \mathsf{S})(\text{ATT}_{\mathcal{A}}(T) \wedge \text{ATT}_{\mathcal{B}}(T))$ is a $\mathsf{SO}\exists$ formula. Given a Boolean formula φ in CNF having clauses $C = \{\varphi_1, \ldots, \varphi_m\}$, let $\mathcal{A}$ be the RS in the proof of Theorem 4, and let $\mathcal{B}$ be the RS having $(\varnothing, \varnothing, C)$ as its only reaction. Clearly, $\mathcal{B}$ has C as its only fixed point attractor. Hence, $\mathcal{A}$ and $\mathcal{B}$ share a fixed point attractor iff φ is satisfiable. This proves that the problem is NP-hard. □

Perhaps surprisingly, verifying if two systems share all their fixed point attractors goes one level up in the polynomial hierarchy *w.r.t.* the other problems pertaining fixed point attractors, thus providing a further example of a natural Π_2^{P}-complete problem.

Theorem 5. *Given two RS $\mathcal{A}$ and $\mathcal{B}$ with a common background set S, it is Π_2^{P}-complete to decide whether $\mathcal{A}$ and $\mathcal{B}$ share all their fixed point attractors.*

Proof. The problem lies in Π_2^{P}, since $(\forall T \subseteq \mathsf{S})(\text{ATT}_{\mathcal{A}}(T) \Leftrightarrow \text{ATT}_{\mathcal{B}}(T))$ is a $\mathsf{SO}\forall\exists$ formula. We prove the Π_2^{P}-hardness by reduction from the $\forall\exists\mathsf{SAT}$ problem [17]. Let $V = \{x_1, \ldots, x_n\}$, $V_1 \subseteq V$, and $V_2 = V - V_1$; let $(\forall V_1)(\exists V_2)\varphi$ be a quantified Boolean formula over V with $\varphi = \varphi_1 \wedge \cdots \wedge \varphi_m$ quantifier-free and in CNF. Finally, let $V_1' = \{x' : x \in V_1\}$ and $C = \{\varphi_1, \ldots, \varphi_m\}$. Define a RS $\mathcal{A}$ with background set $S = V \cup V_1' \cup C \cup \{\spadesuit, \clubsuit\}$ and the reactions

$$(\{x\}, C \cup V_1' \cup \{\spadesuit, \clubsuit\}, \{\varphi_j\}) \quad \text{for } 1 \leq j \leq m,\ x \in \text{pos}(\varphi_j) \tag{13}$$

$$(\varnothing, \{x\} \cup C \cup V_1' \cup \{\spadesuit, \clubsuit\}, \{\varphi_j\}) \quad \text{for } 1 \leq j \leq m,\ x \in \text{neg}(\varphi_j) \tag{14}$$

$$(\{x\}, C \cup V_1' \cup \{\spadesuit, \clubsuit\}, \{x'\}) \quad \text{for } x \in V_1 \tag{15}$$

$$(\text{neg}(\varphi_j), \text{pos}(\varphi_j) \cup C \cup V_1' \cup \{\spadesuit, \clubsuit\}, \{\spadesuit\}) \quad \text{for } 1 \leq j \leq m \tag{16}$$

$$(\{\spadesuit\}, \varnothing, \{\clubsuit\}) \tag{17}$$

$$(\{\clubsuit\}, \{\spadesuit\}, \{\spadesuit\}) \tag{18}$$

$$(C, V \cup \{\spadesuit, \clubsuit\}, C) \tag{19}$$

$$(\{x'\} \cup C, V \cup \{\spadesuit, \clubsuit\}, \{x'\}) \quad \text{for } x' \in V_1'. \tag{20}$$

When the current state of $\mathcal{A}$ is $X \subseteq V$, the reactions of types (13) and (14) produce the set of clauses satisfied by the assignment encoded by X; simultaneously, reactions of type (15) produce "primed" copies of the elements encoding the partial assignment to the universally quantified variables of φ (while the elements encoding the partial assignment to the existentially quantified variables are implicitly discarded). If one of the clauses is not satisfied by X, the corresponding reaction of type (16) is enabled and produces $\spadesuit$. Any state containing $\spadesuit$ or $\clubsuit$ end up in a cycle between $\{\spadesuit\}$ and $\{\clubsuit\}$ by means of reactions (17) and (18). If all clauses appear in the current state, they are preserved by reaction (19), together with any element of V_1' (reactions of type (20)). The inhibitors of reactions (13)–(20) ensure that "bad" states, *i.e.*, those not of the form $X \subseteq V$ or $C \cup U$ with $U \subseteq V_1'$, are mapped to $\{\spadesuit\}$, $\{\clubsuit\}$, or $\varnothing$ (which is a subset of V).

Summarising, the RS $\mathcal{A}$ defines the result function

$$\mathrm{res}_{\mathcal{A}}(T) = \begin{cases} C \cup U & \text{where } U = \{x' \in V_1' : x \in V_1 \cap T\} \text{ if } T \subseteq V \text{ and } T \vDash \varphi \\ T & \text{if } T = C \cup U \text{ with } U \subseteq V_1' \\ D \cup \{\spadesuit\} & \text{if } T \subseteq V,\ D \subsetneq C \text{ and } T \text{ satisfies the clauses in } D \\ & \quad \text{but not the clauses in } C - D \\ \{\spadesuit\} & \text{if } \clubsuit \in T \text{ and } \spadesuit \notin T \\ \{\clubsuit\} & \text{if } \spadesuit \in T \\ \varnothing & \text{otherwise.} \end{cases}$$

The RS $\mathcal{A}$ admits $2^{|V_1|}$ fixed points, all of them of the form $C \cup U$ with $U \subseteq V_1'$; a state of this form is an attractor iff there exists a state $X = \{x : x' \in U\} \cup Y$, with $Y \subseteq V_2$, such that $X \vDash \varphi$. Hence, $\mathcal{A}$ has $2^{|V_1|}$ fixed point attractors iff $(\forall V_1)(\exists V_2)\varphi$ is valid. Let $\mathcal{B}$ be a RS having the reactions $(\{x'\}, \varnothing, \{x'\})$ for $x' \in V_1'$, and $(\varnothing, \varnothing, C)$. The result function of $\mathcal{B}$ is $\mathrm{res}_{\mathcal{B}}(T) = C \cup (T \cap V_1')$, having the same fixed points as $\mathcal{A}$; each fixed point of $\mathcal{B}$ is an attractor, since we have $\mathrm{res}_{\mathcal{B}}(C \cup U \cup \{\spadesuit\}) = C \cup U$ for each $U \subseteq V_1'$. Hence, the RS $\mathcal{A}$ and $\mathcal{B}$ have the same fixed point attractors iff $(\forall V_1)(\exists V_2)\varphi$ is valid. Since the mapping $\big((\forall V_1)(\exists V_2)\varphi\big) \mapsto (\mathcal{A}, \mathcal{B})$ is computable in polynomial time, the problem is Π_2^{P}-hard. □

6 Conclusions

In this paper we have studied the complexity of checking the presence of many different dynamical behaviours of a RS. Deciding if a point is fixed is easy (FO, *i.e.*, FO-uniform AC^0), however it gets increasingly hard to determine the existence of a fixed point (NP-complete), or if two RS have the same fixed points (coNP-complete). When considering fixed point attractors, the majority of the problems are NP-complete, but determining if two RS share all fixed point attractors is one of the few "natural" examples of a Π_2^{P}-complete problem.

The paper discloses many possible research directions. First of all, it would be very interesting to understand why the comparison of local attractors is a Π_2^{P}-complete problem and if there are other relevant dynamical properties that populate (supposedly) different levels of the polynomial hierarchy. We are also investigating the complexity of determining the existence of *global* attractors, cycles, and attractor cycles.

The RS studied in the paper are deterministic. However many significant modelling questions involve RS where extra entities are provided externally (*i.e.*, RS with *context*). These RS are, in some sense, non-deterministic, since starting from the same initial state, we can obtain different dynamics depending on the context. It is interesting to understand how the complexity of decision problems about dynamics changes in this case.

Another promising research direction is the study of minimality, *i.e.*, understanding what is the complexity of the problem of deciding if a given RS is the minimal one (*e.g.*, with respect to the number of reactions) having a given dynamical behaviour.

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