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Irreducible reaction systems and reaction system rank

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ABSTRACT

Reaction systems, introduced by Ehrenfeucht and Rozenberg, are a simple yet versatile model of computation inspired by biochemical reactions in living cells. This contribution falls under one of the active research lines that studies the mathematical nature of subset functions specified by reaction systems, also called *rs functions*. We introduce the concept of *irreducibility* for reaction systems and also *reaction system rank* for rs functions. Apart from some elementary results and basic analysis, the paper focuses on the bounds of reaction system rank. It is found that for every background set, the upper limit of reaction system rank (for all corresponding rs functions, as well as for those that are bijective) is attainable.

1. Introduction

Reaction systems, introduced in 2007 by Ehrenfeucht and Rozenberg [5], are formal models of computations motivated by biochemical reactions taking place in the living cell. The central idea is that the interaction between individual reactions are regulated according to the mechanisms of facilitation and inhibition. The setup of reaction systems allows for various extensions and has led to various diverse research lines. There has been a significant spike of contributions tracing back to reaction systems in the last few years. For an early survey of reaction systems, we refer the reader to [1].

Fix a nonempty background set S. Formally, a reaction system is a set of reactions $a = (R, I, P)$, where R, I, and P are the reactant set, inhibitor set, and product set of a, all of which are subsets of S with R and I being disjoint. A state is a subset of S. For a reaction a to be enabled by a state, every element of the reactant set must be present and no element of the inhibitor set can be present. If a state is enabled by a, then the elements of the product set of a are included in the next state. Hence, every reaction system specifies a state transition function.

An active research line initiated in [4] pertains to the mathematical study of the state transition functions. Reaction systems have been classified according to the bound on the number of resources in each of its reactions. The theory of functions defined by minimal reaction systems, where the reactant set and inhibitor set are singletons, has received remarkable interest [3,8–11,13]. Few other works (not necessarily all) that pursue this type of purely mathematical study are [6,7,12].

This contribution adds to the list of work above. We introduce two new mathematical concepts regarding reaction systems: irreducibility and reaction system rank. A reaction system is irreducible iff no proper subset of its set of reactions

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leads to the same function from 2^S into 2^S. Meanwhile, the reaction system rank measures the complexity of these functions (called rs functions). Unlike minimal reaction systems, it is based on the size of the set of reactions.

The remainder of this paper is structured as follows. Section 2 provides the basic terminology and preliminaries for reaction systems. Irreducibility for reaction systems is introduced and studied in Section 3. The next section deals with reaction system rank and some elementary results regarding its bounds are presented. The subsequent section is dedicated to our main result that guarantees the existence of bijective rs functions attaining the largest possible reaction system rank. In the final section, we highlight a couple of future directions.

2. Basic notions of reaction systems

The set of positive integers is denoted by $\mathbb{N}$. The cardinality of an arbitrary finite set A is denoted by $|A|$. A function f is bijective iff it is one-to-one and onto and its range is denoted by $\mathrm{rng}(f)$.

For an arbitrary set S, let 2^S denote the power set of S and let Φ_S denote the null function $\Phi_S : 2^S \to 2^S$ defined by $\Phi_S(X) = \emptyset$ for all $X \subseteq S$.

Definition 2.1. Suppose S is a finite nonempty set. A *reaction in* S is a triple $a = (R_a, I_a, P_a)$, where R_a and I_a are disjoint (possibly empty) subsets of S and P_a is a nonempty subset of S. The sets R_a, I_a, and P_a are the *reactant set*, *inhibitor set*, and *product set* respectively.

Definition 2.2. A *reaction system* is a pair $\mathcal{A} = (S, A)$, where S is a finite nonempty *background set* and A is a (possibly empty) set of reactions in S.

Definition 2.3. Suppose $\mathcal{A} = (S, A)$ is a reaction system. The function $\mathrm{res}_{\mathcal{A}} : 2^S \to 2^S$ specified by $\mathcal{A}$ is given by

$$\mathrm{res}_{\mathcal{A}}(X) = \bigcup_{\substack{a \in A \\ R_a \subseteq X, I_a \cap X = \emptyset}} P_a, \quad \text{for all } X \subseteq S.$$

Suppose a is a reaction in S and $X \subseteq S$. If $R_a \subseteq X$ and $I_a \cap X = \emptyset$, then we say that a is *enabled by* X. Hence, $\mathrm{res}_{\mathcal{A}}(X)$ is actually the union of the product sets P_a for those reactions a that are enabled by X. Obviously, the set union is empty if no reaction is enabled by X.

When S is understood or fixed, we may write res_A for $\mathrm{res}_{\mathcal{A}}$. For simplicity, we write $\mathrm{res}_a(X)$ for $\mathrm{res}_{\{a\}}(X)$. Thus $\mathrm{res}_A(X) = \bigcup_{a \in A} \mathrm{res}_a(X)$.

Note that if a is enabled by X and $R_a \subseteq Y \subseteq X$, then a is also enabled by Y. Additionally, if A is empty, then $\mathrm{res}_{\mathcal{A}} = \Phi_S$.

The following terminology was first coined by Salomaa in [8].

Definition 2.4. Suppose $\mathcal{A} = (S, A)$ is a reaction system. A reaction a in S is *maximally inhibited* iff $I_a = S \setminus R_a$. We say that $\mathcal{A}$ is *maximally inhibited* iff every $a \in A$ is maximally inhibited.

Every function specified by a reaction system can be canonically specified by one that is maximally inhibited. In fact, if S is a finite nonempty set and $f : 2^S \to 2^S$, then $f = \mathrm{res}_A$, where

$$A = \{ (X, S \setminus X, f(X)) \mid f(X) \neq \emptyset \text{ and } X \subseteq S \}.$$

Due to this, we give the following definition.

Definition 2.5. Suppose S is a finite nonempty set. Every function $f : 2^S \to 2^S$ is called an *rs function over* S. It is *null* iff $f = \Phi_S$.

Remark 2.6. In the literature, it is often assumed that the reactant sets and inhibitor sets are nonempty. Hence, in this case, an rs function over S is any function $f : 2^S \to 2^S$ satisfying $f(\emptyset) = f(S) = \emptyset$. However, accordingly with Definition 2.1, we do not adopt here this assumption.

Definition 2.7. Suppose $\mathcal{A}$ and $\mathcal{B}$ are reaction systems. We say that $\mathcal{A}$ and $\mathcal{B}$ are *functionally equivalent* iff $\mathrm{res}_{\mathcal{A}} = \mathrm{res}_{\mathcal{B}}$.

Remark 2.8. Functionally equivalent reaction systems must have the same background set. Hence, for a fixed background set S, functional equivalence can be viewed as an equivalence relation between sets of reactions in S. Furthermore, if (S, A) and (S, B) are functionally equivalent reaction systems and $S \subseteq T$, then (T, A) and (T, B) are also functionally equivalent.

The following terminology was introduced in [7].

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