Theoretical Computer Science 598 (2015) 138–149

Contents lists available at ScienceDirect

Theoretical Computer Science

www.elsevier.com/locate/tcs

Reaction systems and extremal combinatorics properties ☆

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ARTICLE INFO

Article history:
Received 17 August 2014
Received in revised form 18 May 2015
Accepted 1 June 2015
Available online 9 June 2015
Communicated by N. Jonoska

Keywords:
Reaction systems
Combinatorics
Natural computing

ABSTRACT

Extremal combinatorics is the study of the size that a collection of objects must have in order to certainly satisfy a given property. Reaction systems are a recent formalism for computation inspired by chemical reactions. This work is a first contribution to the study of the behavior of large reaction systems by means of extremal combinatorics. We define several different properties that capture some basic and dynamical behaviors of a reaction system and we prove that they must necessarily be satisfied if the system is large enough. Explicit bounds and formulae are also provided.

1. Introduction

In 2004, Ehrenfeucht and Rozenberg introduced *Reaction systems (RS)*: a new interesting computation model inspired by chemical reactions [6]. Similarly to their real counterparts, RS reactions need a set of chemicals (the *reactants*) to act on and either can be inhibited by other chemicals (the *inhibitors*) or produce some *products*. Formally, a *reaction* consists of these three sets, each of which is coded as a set of symbols and an RS is a set of reactions over a common set of symbols (the *entities*). The size of such a system is simply defined as the number of reactions of which it is composed.

This work provides a first study on the behavior of large RS. For the first time (at our knowledge) concepts from extremal combinatorics are applied to the field of RS. Other works on RS dynamics have also been carried on adopting a completely different point of view [5]. Indeed, the authors investigated the properties of randomly generated RS. Conversely, here we focus on some property P and the goal is to find minimal bounds on the size of RS such that all RS of larger size exhibit P.

Combinatorial statements arise almost naturally in many fields. Those about the properties that a certain structure can exhibit when its size increases are particularly important. A famous statement of this kind is, for example, the *Ramsey theorem*, that states that for every $k \in \mathbb{N}$, any large enough complete two-colored graph has a monochromatic subgraph of k nodes. Other examples come from the most different mathematical structures. These statements can be presented in many ways. One can either point out the existence of a size bound after which a certain property holds (a more *Ramsey*-like view), or try to find the exact value of this bound or, at least, obtain some information on its order of magnitude (an extremal combinatorics point of view). To prove statements of extremal combinatorics a large body of work regarding proof techniques has been produced, ranging from various counting techniques to combinatorial proofs and linear algebra methods. Since it is impossible to give a detailed account of all the results and the techniques, we refer the reader to specific books (see, for example, [11] for extremal combinatorics and [10] for Ramsey theory).

☆ This is an extended and improved version of the work presented at LATA 2014 conference [3].

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http://dx.doi.org/10.1016/j.tcs.2015.06.001
0304-3975/

This paper studies the minimal size after which a reaction system:

- necessarily exhibits a non-sequential behavior.
- always exhibits a non-sequential behavior.
- includes two reactions such that the reactants of one of them inhibit the other.
- necessarily has a reaction that produces the inhibitors of another reaction.
- can be substituted by a smaller reaction system with the same dynamics.
- cannot be written as the union of two reaction systems with a disjoint set of entities.

These properties help to clarify the limits in size and in parallelism that are inherent in the definition of RS. In a sense they concern the "static" behavior of an RS. However, since RS can be used to model and study biological processes, determining if a particular biological system exhibits a certain behavior is an important task with potential real-life impacts [2,1].

Since RS are finite systems (i.e., they can take only a finite number of distinct states), it is clear that their dynamics is eventually periodic. However, both the period and the preperiod can be of exponential size w.r.t. the description of the RS. As a consequence, decision problems about the dynamics of RS often belong to high complexity classes [8,4]. In this paper, we try to quantify the minimal size which an RS should have to have some given dynamical property. This, in a sense gives a bound for the solution set of such decision problems.

More precisely, we show how large an RS must be to exhibit a controlled dynamical behavior where the control specifies a bound on the number of its attractors, the length of the corresponding cycles, and the length of the transients of all its dynamical evolutions.

All the results in the paper are stated for both the definitions of RS that can be found in literature. Indeed, one of them disallows empty reactant, inhibitor, and product sets and, due to this condition, it is more suitable for modeling biological systems [1,2]. The second one has no such restrictions and it is more handy for theoretical studies of RS, for example regarding the computational complexity of their dynamical properties [9,8]. These two definitions are, in most cases, equivalent. However, as to extremal combinatorics properties, the bounds are different since more reactions are allowed in the latter definition with respect to the former. Therefore, we provide bounds for both definitions.

Remark that many of the results obtained in this paper can also be restated as Ramsey-like statements (i.e., in terms of presence of an "ordered" substructure inside a large enough structure).

The paper is structured as follows. The next section recalls basic notions about RS. Section 3 contains the main results about basic properties while Section 4 concerns the dynamical behavior of reaction systems. Further remarks are provided in Section 5.

2. Reaction systems

In this section, we give the basic notions about reaction systems, including the concepts of dynamics and equivalence. Most of notations are taken from [7].

2.1. Basics of reaction systems

We first recall the main concept of reaction. Inspired by real chemical reactions, it comprises three sets corresponding to the reactants, the inhibitors, and the products of the reaction.

Definition 1. A *reaction* $\mathsf{a} = (R_\mathsf{a}, I_\mathsf{a}, P_\mathsf{a})$ is a triple of three non-empty and finite sets such that $R_\mathsf{a} \cap I_\mathsf{a} = \emptyset$. R_a is called the set of *reactants*, I_a the set of *inhibitors*, and P_a the set of *products*, respectively. For any finite set S, we say that a is a reaction in S if $R_\mathsf{a} \subseteq S$, and $I_\mathsf{a} \subseteq S$, and $P_\mathsf{a} \subseteq S$.

Definition 2. A *generalized reaction* $\mathsf{a} = (R_\mathsf{a}, I_\mathsf{a}, P_\mathsf{a})$ is a triple of finite sets, where R_a, I_a, and P_a are called *reactants*, *inhibitors*, and *products*, respectively.

The *set of all possible reactions (resp., generalized reactions) in a finite set* S is denoted by $rac(S)$ (resp., $rac_g(S)$).

Definition 3. A *Reaction System (RS)* (resp., a *generalized Reaction System (RS_g)*) is a pair $\mathcal{A} = (S, A)$, where S is a finite set of symbols and $A \subseteq rac(S)$ (resp., $A \subseteq rac_g(S)$). The set S is called the background of $\mathcal{A}$.

Let S be a finite set. For any $T \subseteq S$ and any reaction $\mathsf{a} \in rac(S)$, we say that a *is enabled by* T if $R_\mathsf{a} \subseteq T$ and $I_\mathsf{a} \cap T = \emptyset$. The *result* $res_\mathsf{a}(T)$ *of a reaction* $\mathsf{a} \in rac(S)$ *on a set* $T \subseteq S$ is defined as $res_\mathsf{a}(T) = P_\mathsf{a}$ if a is enabled by T, and $res_\mathsf{a}(T) = \emptyset$ otherwise. The previous notion extends naturally to sets of reactions: the *result set of* A *on a subset* $T \subseteq S$ is $res_A(T) = \bigcup_{\mathsf{a}\in A} res_\mathsf{a}(T)$. For any $A \subseteq rac(S)$, the *reactant, inhibitor, and product set of* A are $R_A = \bigcup_{\mathsf{a}\in A} R_\mathsf{a}$, $I_A = \bigcup_{\mathsf{a}\in A} I_\mathsf{a}$, and $P_A = \bigcup_{\mathsf{a}\in A} P_\mathsf{a}$, respectively. Furthermore, we say that A *is enabled by* T if every reaction $\mathsf{a} \in A$ is enabled by T.

The *result set of an RS* $\mathcal{A} = (S, A)$ *on a subset* $T \subseteq S$ is $res_\mathcal{A}(T) = res_A(T)$. Denote by $\mathcal{P}(S)$ the collection of all subsets of S. The notion of result set defines the *result function* $res_\mathcal{A} : \mathcal{P}(S) \to \mathcal{P}(S)$ associating every element $T \in \mathcal{P}(S)$ with the