Theoretical Computer Science ••• (••••) •••–•••

Contents lists available at ScienceDirect

Theoretical Computer Science

www.elsevier.com/locate/tcs

A graph isomorphism condition and equivalence of reaction systems ☆

Daniela Genova [a], Hendrik Jan Hoogeboom [b], Nataša Jonoska [c,*]

[a] Department of Mathematics and Statistics, University of North Florida, Jacksonville, USA
[b] LIACS, Leiden University, The Netherlands
[c] Department of Mathematics and Statistics, University of South Florida, Tampa, USA

ARTICLE INFO

Article history:
Received 7 January 2017
Received in revised form 30 April 2017
Accepted 3 May 2017
Available online xxxx

Keywords:
Directed graphs
Graph isomorphism
Graphs on posets
Dynamics of reaction systems
Equivalence of reaction systems

ABSTRACT

We consider global dynamics of reaction systems as introduced by Ehrenfeucht and Rozenberg. The dynamics is represented by a directed graph, the so-called transition graph, and two reaction systems are considered equivalent if their corresponding transition graphs are isomorphic. We introduce the notion of a skeleton (a one-out graph) that uniquely determines a directed graph. We provide the necessary and sufficient conditions for two skeletons to define isomorphic graphs. This provides a necessary and sufficient condition for two reactions systems to be equivalent, as well as a characterization of the directed graphs that correspond to the global dynamics of reaction systems.

1. Introduction

Determining whether two graphs are isomorphic is one of the archetypical problems in graph theory and plays an important role in many applications and network analysis problems. Although there have been significant advances for this problem in the past year [1], the problem remains difficult. On the other side, often in network analysis, graphs are partitioned in so called 'modules' where each vertex in a module is adjacent to the same set of vertices outside the module [9]. Modules in directed graphs are defined as sets of vertices that have incoming and outgoing edges from, and to, the same vertices outside the module and it is shown that modular decompositions can be performed in linear time [11]. In this paper we study graph isomorphism through a variation of this notion, where we consider vertices that have the "same" incoming edges, and we call such vertices "companions". These vertices are precisely those that belong to the same region in the Venn diagram constructed out of the family of out-sets (an out-set for v is the set of vertices that have incoming edges starting at v). We further define a "skeleton" of a graph $G = (V, E)$ as a one-out graph over a set V such that the set of vertices that have non-zero in-degree are representatives of the family of out-sets. A skeleton defines uniquely a directed graph and we characterize skeletons of isomorphic graphs. Skeletons of isomorphic graphs are called "companion skeletons". In particular, skeleton edges swapped at companion vertices produce companion skeletons. This observation allows characterizations of reaction systems (described below) that exhibit the same global dynamical behavior.

A formal description of biochemical interactions within a confined region bounded with a porous membrane that can interact with the environment has been introduced in [5], see [2] for an overview of the theory. This formal model, called

☆ This work has been supported in part by the NSF grant CCF-1526485 and NIH grant R01 GM109459.
* Corresponding author.
E-mail address: jonoska@math.usf.edu (N. Jonoska).

http://dx.doi.org/10.1016/j.tcs.2017.05.019
0304-3975/© 2017 Elsevier B.V. All rights reserved.

"reaction systems", is based on the idea that each reaction depends on the presence of a compound of enzymes, or facilitators, and the absence of any other control substance that inhibits the process. It is assumed further that the reaction is enabled only if the region contains all of the enabling ingredients and none of the inhibitors. In addition, if some ingredients are present in the system, the model allows their presence to be sufficient to enable all reactions where they participate. Formally, a reaction is modeled by a triple of sets (reactants, inhibitors, results) while the reaction system then represents a set of such triples. In each step, the system produces resulting elements according to the set of reactants that are enabled. It is further assumed that there is a universal set of elements that can enter the system from the outside environment and interact with the reactants at any given time. Several studies have addressed the question of the dynamics of the system (the step by step changes of the states of the system), such as reachability [4], convergence [8], fixed points and cycles [7,6]. It has been observed that the complexity of deciding existence of certain dynamical properties falls within PSPACE (reachability) or NP-completeness (fixed points and fixed point attractors). In all of these studies, however, the changes in the dynamics through inclusion of new elements entering from the outside environment has not been considered. We call this condition of no outside involvement within the system as a 0-context reaction system. In this paper we study the relationship between the dynamics of the 0-context reaction systems and the global dynamics of the reaction system that depends on the environmental context. We observe that quite different dynamical properties of 0-context reaction systems produce equivalent global dynamics.

We represent the dynamics of a reaction system as a directed graph where each vertex is a state of the system represented as a set of elements present at the system at a given time. A directed edge from a vertex terminates at a vertex representing the new state of the system after all reactions enabled at the origin, with possible additions from the outside environment, are performed. In this way, the graph of the 0-context reaction system is a one-out graph (a skeleton) and is a subgraph of the graph of the full dynamics of the system. We characterize the graphs representing the global dynamics of reaction systems and show that two reaction systems are equivalent if their 0-context graphs are companion skeletons.

2. Subsets and companions

We denote $[n] = \{0, 1, \ldots, n-1\}$. The power set of a set A is denoted by 2^A. The number of elements of a finite set A is denoted by $|A|$ and is called the *size* of A. Given a function $f : X \to Y$, the natural equivalence on X defined by f is denoted with $\ker f$, i.e., $x \ker f y$ if and only if $f(x) = f(y)$. For $x \in X$ the equivalence class of $\ker f$ is denoted $[x]_f$. For a finite set V, let $\mathcal{O} \subseteq 2^V$ be a family of subsets of V. We say that $\mathcal{O}$ is a family of sets with domain V. The elements in V that appear in the same region of the Venn diagram for $\mathcal{O}$ are "companions" with respect to $\mathcal{O}$. Formally, let $\mathcal{N}_{\mathcal{O}}(x) = \{X \in \mathcal{O} \mid x \in X\}$ be the subfamily containing all sets that include x and $\mathcal{N}^c_{\mathcal{O}}(x)$ its complement in $\mathcal{O}$, the subfamily of those sets that do not contain x. We call $\mathcal{N}_{\mathcal{O}}(x)$ the *neighborhood* of x.

Definition 2.1. Let V be a finite set and $\mathcal{O} \subseteq 2^V$ be a family of subsets of V. Two elements $x, y \in V$ are *companions with respect to* $\mathcal{O}$ if $\mathcal{N}_{\mathcal{O}}(x) = \mathcal{N}_{\mathcal{O}}(y)$. We write $x \sim_{\mathcal{O}} y$ and denote the equivalence class of x by $C_{\mathcal{O}}(x)$. The set $C_{\mathcal{O}}(x)$ is called a *companion set*.

Thus, the equivalence class of every element $x \in V$, the set of companions of x relative to $\mathcal{O}$, is the intersection of all sets in $\mathcal{O}$ that include x minus the union of the remaining sets in $\mathcal{O}$, i.e. $C_{\mathcal{O}}(x) = \bigcap \mathcal{N}_{\mathcal{O}}(x) \setminus \bigcup \mathcal{N}^c_{\mathcal{O}}(x)$. The same equivalence based on neighborhoods of elements with respect to a family was also used in [3] where authors study activity regions for a set of neurons and the convexity of these regions was considered. A special case is when $\mathcal{N}_{\mathcal{O}}(x) = \varnothing$, i.e., when $x \notin \bigcup \mathcal{O}$, in which case it is in the outer region, $V \setminus (\bigcup \mathcal{O})$ denoted by $\left(\bigcup \mathcal{O}\right)^c$, of the Venn diagram for $\mathcal{O}$. That is, by convention, $\bigcap \mathcal{N}_{\mathcal{O}}(x) = \bigcap \varnothing = V$ and $C_{\mathcal{O}}(x) = \left(\bigcup \mathcal{O}\right)^c$.

The converse also holds. Any intersection of sets in $\mathcal{P} \subseteq \mathcal{O}$ minus the union of the remaining sets $\mathcal{P}^c = \mathcal{O} \setminus \mathcal{P}$ forms an equivalence class $C_{\mathcal{P}}$, provided it is non-empty. More precisely, any non-empty $C_{\mathcal{P}} = \bigcap \mathcal{P} \setminus \bigcup \mathcal{P}^c$ for some $\mathcal{P} \subseteq \mathcal{O}$ coincides with $C_{\mathcal{O}}(x)$ for some $x \in V$. Assuming $x \in C_{\mathcal{P}}$, it implies $x \in X$ for every $X \in \mathcal{P}$ and $x \notin Y$ for every $Y \in \mathcal{P}^c$. Hence, $x \in \bigcap \mathcal{N}_{\mathcal{O}}(x) \setminus \bigcup \mathcal{N}^c_{\mathcal{O}}(x) = C_{\mathcal{O}}(x)$ and $C_{\mathcal{P}} \subseteq C_{\mathcal{O}}(x)$. Conversely, if $y \in C_{\mathcal{O}}(x)$ then $y \in \bigcap \mathcal{N}_{\mathcal{O}}(x)$ which is precisely $\bigcap \mathcal{P}$ and $y \notin \bigcup N^c_{\mathcal{O}}(x) = \bigcup \mathcal{P}^c$ for $\mathcal{P} = \mathcal{N}_{\mathcal{O}}(x)$ and hence $C_{\mathcal{O}}(x) \subseteq C_{\mathcal{P}}$. Thus, $C_{\mathcal{P}} = C_{\mathcal{O}}(x)$.

Therefore, every equivalence class C of $\sim_{\mathcal{O}}$ is characterized by a subset $\mathcal{P} \subseteq \mathcal{O}$, its neighborhood, such that $C = \bigcap \mathcal{P} \setminus \bigcup \mathcal{P}^c$. In general, not every $\mathcal{P} \subseteq \mathcal{O}$ defines an equivalence class, i.e., $\bigcap \mathcal{P} \setminus \bigcup \mathcal{P}^c$ might be empty. This is the case when the corresponding region of the Venn diagram of $\mathcal{O}$ is empty.

For a family of sets $\mathcal{O}$ we denote with $\mathcal{O}^\cap$ the smallest family of sets that contains $\mathcal{O}$ and is closed under intersection. We say that $\mathcal{O}^\cap$ is the *intersection* closure of $\mathcal{O}$. If $\mathcal{O} = \mathcal{O}^\cap$ we say that $\mathcal{O}$ is *intersection closed*.

Example 2.1. Consider the finite set $V = \{1, 2, \ldots, 8\}$ and the family of subsets $\mathcal{O} \subseteq 2^V$ given by $\mathcal{O} = \{\{1, 2, 3, 4\}, \{4, 5\}, \{5\}\}$. Then $\mathcal{O}^\cap = \mathcal{O} \cup \{\{4\}\}$. Note that $C_{\mathcal{O}}(1) = \bigcap \mathcal{N}_{\mathcal{O}}(1) \setminus \bigcup \mathcal{N}^c_{\mathcal{O}}(1) = \{1, 2, 3, 4\} \setminus (\{4, 5\} \cup \{5\}) = \{1, 2, 3\} = C_{\mathcal{O}}(2) = C_{\mathcal{O}}(3)$ and $C_{\mathcal{O}}(4) = \{4\}$. Thus, the family $\mathcal{O}$ defines the following companion sets: $\{1, 2, 3\}$, $\{4\}$, $\{5\}$, and $\{6, 7, 8\}$, where each nonempty region in the corresponding Venn diagram is a companion set.

In the sections that follow we use a correspondence of families of sets, that have the same sizes of the sets as well as their intersections.

Please cite this article in press as: D. Genova et al., A graph isomorphism condition and equivalence of reaction systems, Theoret. Comput. Sci. (2017), http://dx.doi.org/10.1016/j.tcs.2017.05.019