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Predictors for flat membrane systems

Roberto Barbuti, Roberta Gori *, Paolo Milazzo

Dipartimento di Informatica, Università di Pisa, Largo Pontecorvo 3, 56127 Pisa, Italy

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ABSTRACT

In this paper we investigate dynamic causalities in membrane systems by proposing the concept of "predictor", originally defined in the context of the reaction systems by Brijder, Ehrenfeucht and Rozenberg. The goal is to characterise sufficient and necessary conditions for the presence of a multiset of molecules of interest in the configuration of a P system at a given evolution step (independently from the non-deterministic choices taken). These conditions can be used to study causal relationships between molecules and, therefore, to predict some aspects of future development of multiset rewriting systems.

To achieve this goal, we introduce the new concept of "multiset pattern" representing a logical formula on multisets. A *sufficient predictor* can be expressed as a pattern characterising initial multisets that *will surely evolve*, after the given number of evolution steps, into a multiset containing the molecules of interest. On the other hand, a *necessary predictor* models initial multisets that *may evolve* after the given number of evolution steps, into a multiset containing the molecules of interest. Necessary predictors can be used to characterise initial multisets that *will surely not evolve* (in the required number of steps) into a multiset that contains such molecules. We inductively define operators able to compute these predictors.

The patterns obtained from our operators are sound (sufficient or necessary) predictors, but, in general, they are not complete.

1. Introduction

The understanding of causal relationships among the events happening in a biological (or bio-inspired) system is an issue widely investigated in the context of both systems biology (see e.g. [1–3]) and natural computing (see e.g. [4]).

In [5] Brijder, Ehrenfeucht and Rozenberg initiate a study on *causalities* in reaction systems [6,7]. Causalities deal with the ways entities of a reaction system influence each other. In [5], both static/structural causalities and dynamic causalities are discussed, introducing the idea of *predictors*. A predictor can be used to determine whether a molecule of interest s will be produced after k execution steps of the reaction system, without executing the system itself.

In reaction systems the environment is the only source of non-determinism. Knowledge about the molecules which will be provided at each step by the environment is required to determine whether a molecule s will be produced after k steps. Not all molecules are relevant for the production of s. On the basis of these two observations, a predictor is defined as the subset of molecules Q whose supply by the environment need to be observed in order to determine whether s will be produced or not after k steps.

* Corresponding author.
E-mail addresses: barbuti@di.unipi.it (R. Barbuti), gori@di.unipi.it (R. Gori), milazzo@di.unipi.it (P. Milazzo).

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In [8–10], the idea of predictors was enhanced by defining the notion of *formula based predictor*. A formula based predictor consists in a propositional logic formula to be satisfied by the sequence of sets of molecules that the environment provides to the reaction system. This logic formula clearly discriminates between the cases in which a particular molecule s will be produced after a given number of steps and the cases in which it will not.

P systems [11,12] are much more powerful and complex than reaction systems. They are based on multisets rather than sets and evolution rules are applied with *maximal parallelism* and with a non-deterministic competition for reactants.

The computational behaviour of a P system is determined only by the initial multiset and by the non-deterministic choices made at each maximally parallel step. In this context, a notion of predictor may correspond to a logical formula to be satisfied by the initial multiset (representing either a *sufficient condition* or a *necessary condition*) for the molecules of interest to be present after a given number of evolution steps. Due to the intrinsically non-deterministic nature of P systems, sufficient and necessary conditions have to be dealt with separately.

Example 1.1. For an intuition, consider the following rewriting rules:

$$r_0: \quad A \to C \qquad r_1: \quad A \to B \qquad r_2: \quad D \to C$$

forming a maximally parallel multiset rewriting system. Assume we are interested in the presence of molecule C after one step of rewriting. If we want to be sure that molecule C will be present after one step we have two possibilities: either C or D have to belong to the initial multiset. Having molecule A in the initial multiset is not sufficient to ensure that molecule C will be produced after one evolution step. Indeed, if rule r_1 is applied the initial multiset does not evolve in one step into a multiset containing molecule C. Therefore, if we want to devise sufficient conditions for the presence of molecule C after one step, we need to characterise in some way all initial multisets containing molecule C or D. On the other hand, if a multiset after one evolution step (from the initial one) contains molecule C then we have three possible cases, either the initial multiset already contained molecule C or the initial multiset contained molecule A or molecule D. Hence, if we are interested in the necessary condition for the presence of molecule C after one step, we have to characterise all the initial multiset containing molecule A or C or D.

The previous example shows that, in general, sufficient and necessary conditions do not coincide, and therefore they have to be handled separately. Note that sufficient conditions can be used to determine the multiset of molecules that will *surely* cause the presence of the molecule of interest in the required number of evolution steps, while necessary conditions can be used to determine, by complementation, the multisets that *surely cannot cause* the presence of a molecule of interest in the required number of evolution steps. Therefore, investigating causal dependencies in the previous example, we can say that the presence of C or D in the initial multiset causes the presence of C after one evolution step but the presence of C after one step cannot be caused by an initial multiset that does not contain neither C nor A nor D.

The previous example also shows that while it is quite easy to deal with necessary conditions, dealing with sufficient condition is a complex task because competition on reactants comes into play.

In this paper we propose the notion of *multiset pattern* as a way to express logical formulas on molecules of multisets. Multiset patterns will be used to characterise sufficient and necessary conditions for a molecule (or, in general, for a multiset of molecules) to be present after a given number of steps. We first focus on the pattern that expresses sufficient conditions. If the initial multiset of the P systems satisfies (*matches*) such a pattern, then the multiset of molecules of interest will be *surely* present after k steps; nothing can be said otherwise (it is indeed a sufficient condition). Such pattern will be defined by a recursive operator. We will show that the pattern obtained from the operator will be a sound, but, in general, not a complete predictor. This means that there can be multisets that do not match the pattern, but that still always lead to the presence of the molecules of interest in k steps. However, there might exist special classes of P system for which the sufficient predictor is also complete. In this paper, we investigate the completeness of our sufficient predictor for P systems with non-cooperative rules.

We then focus on the pattern expressing necessary conditions for the presence of the molecules of interest. In this case we have that if the P system leads to a multiset that contains the molecules of interest in the required number of steps then the initial multiset *matches* the pattern expressing necessary conditions. This information can be used to characterise multisets that surely will not evolve in a multiset containing the molecules of interest in the required number of steps. We provide a recursively defined operator that computes such pattern. Once again, we will show that the pattern we compute will be a sound, but, in general, not complete. This means that there can be multisets that do model the pattern, but will not lead to the presence of the molecules of interest in k steps. However, we prove that for P systems with non-cooperative rules our necessary predictor is also complete.

Once defined, patterns expressing sufficient and necessary conditions can be used to discover non-trivial causal relationships among molecules.

Related works Causality properties have been investigated in different contexts. For example, causalities are studied in the context of concurrency theory, systems biology and natural computing. Different notions of causality have been considered such as dependencies between events or between reachable states of the considered system. Moreover, different techniques have been applied to verify causality properties on system models such as static analysis, enhanced semantics and other formal “ad hoc” techniques.

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