

## Complexity of automata network dynamics under structural constraints

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**Spirit** This PhD subject investigates how global dynamical properties emerge from local interactions in automata networks through the lens of computational complexity. Focusing in particular on settings where only the interaction graph is known, it aims to understand the boundary between tractable and hard problems in discrete dynamical systems under structural constraints.

**Automata networks** An automata network is composed of  $n$  automata, where each automaton  $i \in \{1, \dots, n\}$  holds a state among a finite alphabet  $A$  and a *local function*  $f_i : A^n \rightarrow A$  giving its next state provided the current global state of the system. We have a dynamical system  $(A^n, f)$ , where  $f : A^n \rightarrow A^n$  is defined as  $\forall x \in A^n : f(x) = (f_1(x), \dots, f_n(x))$  i.e., all automata update their state in parallel (*synchronous* mode) at each step. Other update policies may be considered (including *non-deterministic* update modes). The graph of  $f$  on vertex set  $A^n$  is its *dynamics*, denoted  $\mathcal{G}_f$  (it has out-degree one in the synchronous case:  $f(x)$  is the unique out-neighbour of  $x$ ). When  $A = \{0, 1\}$ , we have *Boolean automata networks* (BANs). A central object of AN theory is the *interaction graph* denoted  $G_f$ . It has one vertex per automaton, and an arc from  $i$  to  $j$  whenever  $f_j : A^n \rightarrow A$  effectively depends on its  $i$ -th component (formally, if there exist  $x, y \in A^n$  which only differ on  $x_i \neq y_i$  such that  $f_j(x) \neq f_j(y)$ ). The graph  $G_f$  captures the architecture of the network through the mutual influences among automata. Signs may be added to the arcs of  $G_f$ , representing two non-exclusive types of influence: there is a positive (resp. negative) arc from  $i$  to  $j$  whenever there exists  $x, y \in A^n$  which only differ on  $x_i \neq y_i$  such that the sign of  $(y_i - x_i)(f_j(y) - f_j(x))$  is positive (resp. negative).

**Relating the objects  $(f_i)_{i \in [n]}$ ,  $\mathcal{G}_f$  and  $G_f$**  motivates the AN community, with a wide range of applications from biology to sociology and economics [1, 2, 3]. From a practical point of view, computational complexity gives bounds essential to the design of (the most) efficient algorithms solving problems. From a theoretical point of view, it gives a formal meaning of the term “complex system” and its multiple facets. The objects  $\mathcal{G}_f$  and  $G_f$  are graphs encoded in standard manners, and  $(f_i)_{i \in [n]}$  are functions which may be encoded as circuits (algorithms) or truth-tables (on the in-neighbours of  $i$  in  $G_f$ , so with a particular interest in the case where  $G_f$  has bounded in-degree). Classical results of the domain are structural (for example [4, 5, 6, 7] relate properties of  $G_f$  such as the size of feedback arc sets to properties of  $\mathcal{G}_f$  such as its number of fixed points), whereas we propose to understand these relations through the lens of computational complexity theory. This renewed point of view outlines why some structural bounds are still loose despite considerable efforts [8]. We also aim at transferring this knowledge to other models of computation, via strict simulations acting as reductions.

**A metatheorem** has recently been obtained, encompassing at once a large range of developments. Standard dynamical system approaches aim at understanding the dynamics  $\mathcal{G}_f$ , in terms of the local functions  $(f_i)_{i \in [n]}$ . This naturally turns into decision problems of the form: given  $(f_i)_{i \in [n]}$ , does  $\mathcal{G}_f$  have a given property? Many problems can easily be proven to be NP-complete (e.g. the existence of fixed points, and of limit cycles of a given length [9]) or coNP-complete (e.g. injectivity  $\mathcal{G}_f$  [10]).

**Theorem** ([11]). *Given a deterministic AN  $f$  encoded as Boolean circuits, any non-trivial question on  $\mathcal{G}_f$  expressed in first-order graph logic is NP-hard or coNP-hard.*

First-order graph logic (FO) are formulas evaluated on graphs (finite in our setting), constructed with the usual connectives  $\wedge, \vee, \neg, \Rightarrow$  and quantifications  $\exists, \forall$  on vertices. Atoms are built from the signature  $\{=, \rightarrow\}$  where  $x \rightarrow y$  is true when there is an arc from  $x$  to  $y$ . To a FO formula we associate a decision problem. The non-triviality condition asserts that the formula has an infinity of models and an infinity of counter-models, it is optimal because trivial formulas are decided in constant time. The proof techniques combine

tools from finite model theory (such as Ehrenfeucht-Fraïssé games and Hanf-Gaifman locality) with the constructions of discrete dynamical systems.

**The interaction graph as input** Testing whether the dynamics of an AN  $f$  Boolean network satisfy a given property is natural. However, in practice, in many contexts, only very partial information about the network  $f$  is available. For example, it is common that the only available information is the interaction graph  $G_f$ . The information carried by  $G_f$  is weak because the set of ANs whose interaction graph is  $G$  – denoted  $F_q(G)$ , where  $q$  is the size of the alphabet  $A$  – is on average doubly exponential in  $n$ . If only  $G_f$  is known, a natural question is to decide whether there *exists* a network in  $F_q(G)$  whose dynamics satisfies property  $P$ ; one then (abusively) says that  $G$  satisfies  $P$  on the alphabet of size  $q$  and writes  $G \models_q P$ . In this setting  $G$  can satisfy both a property and its negation.

**Research objectives** Although this class of decision problems “to decide if  $G \models_q P$ ” is natural and well-motivated from the perspective of applications, very few results are known. To the best of our knowledge, the only study that systematically addresses this question is [8]. In particular, it is shown that, when  $G$  is signed, deciding if  $G \models_2 P$  is NEXPTIME-complete (respectively NP-complete) when  $P$  expresses “having no fixed point” (respectively “having at least two fixed points”). The contribution of signs is highly significant here: without them, both problems are polynomial-time solvable!

The aim of this PhD project is to go much further in the analysis of this class of decision problems by considering other simple properties (expressible with first-order formulae, as in the metatheorem mentioned above), signed and unsigned interaction graphs, deterministic and non-deterministic dynamics, as well as binary and non-binary alphabets. The general idea is to gain a better understanding of the boundary between properties that are easy to test and those that are computationally hard.

The unsigned case is particularly intriguing and provides an opportunity to outline concrete research directions. In that case, it is difficult to identify properties that are hard, that is, NP-hard or coNP-hard to test. In particular, we do not know if there exists a property  $P$  such that deciding if  $G \models_q P$  is hard for all alphabet sizes  $q$ . Finding such a property should be one of the primary objectives. Another existential question is : do there exist properties  $P$  such that it is hard to decide if  $G \models_2 P$  and hard to decide if  $G \models_2 \neg P$ .

**Collaborations are expected** with researchers from I3S teams MC3 and ALARICE project.

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