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# Intrinsic Universality in Automata Networks I: Families and Simulations.\*

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## Abstract

An automata network (AN) is a finite graph where each node holds a state from a finite alphabet and is equipped with a local map defining the evolution of the state of the node depending on its neighbors. They are studied both from the dynamical and the computational complexity point of view. Inspired from well-established notions in the context of cellular automata, we develop a theory of intrinsic simulations and universality for families of automata networks. We establish many consequences of intrinsic universality in terms of complexity of orbits (periods of attractors, transients, etc) as well as hardness of the standard well-studied decision problems for automata networks (short/long term prediction, reachability, etc). In the way, we prove orthogonality results for these problems: the hardness of a single one does not imply hardness of the others, while intrinsic universality implies hardness of all of them. We also compare our notions of universality to intrinsic universality of cellular automata. This paper is the first of a series of three: in the second one, we develop a proof technique to establish intrinsic universality based on an operation of glueing; in the third one we study the effect of update schedules on intrinsic universality for concrete symmetric families of automata networks.

## 1 Introduction

An automata network is a (finite) graph where each node holds a state from a finite set  $Q$  and is equipped with a local transition map that determines how the state of the node evolves depending on the states of neighboring nodes. Automata networks introduced in the 40s [39] are both a family of dynamical systems frequently used in the modeling of biological networks [50, 34] and a computational model [19, 9, 20, 54, 53]. As such they can exhibit complexity from two very different point of view: complexity of orbits in their phase space (cycles, transient, etc) and computational complexity of canonical problems associated to them (prediction, reachability, etc). An automata network is completely described by its global map  $F : Q^V \rightarrow Q^V$  that defines the collective evolution of all nodes  $V$  of the network. However, this global map hides two fundamental aspects at the heart of automata network literature [13, 18, 10, 2, 21, 1, 48]: the interaction graph (knowing on which nodes effectively depends the behavior of a given node) and the update schedule (knowing in which order and with which degree of synchrony are local transition maps of each node applied). Moreover, when considering computational complexity, the concrete representation of automata networks crucially matters. An arbitrary global map  $F$  requires as much information to be represented as the complete description of its orbits. On the contrary, many standard families of automata networks are actually described concretely by the interaction graph and the parameters of each local transition map (see Section 2.1). We are mainly interested in such natural families with concrete succinct representations and not in arbitrary global maps.

This paper is the first of a series of three that tackles core questions of automata networks theory:

- how dynamical complexity relates to computational complexity in automata networks?

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- what families exhibit maximal complexity in both aspects and what are the key ingredients or sufficient conditions to achieve it?
- how can update schedules compensate for the limitation coming from restrictions and symmetries of a family?
- what hierarchy of different types of update schedules can be established with respect to the rise of complexity when applied to a family?

One of the key concept that we put forward to tackle these questions is that of intrinsic universality of a family, *i.e.* the ability to simulate arbitrary automata networks. In this first paper, we focus on the formalism of universality of families of automata networks and its consequences both for dynamics and computational complexity. The second paper establishes a proof technique for universality based on an operation of glueing of networks and pseudo-orbits. Building upon these tools, the third paper is devoted to update schedules and their key influence on concrete families of automata networks, in particular how a non-universal family can recover universality under a particular update schedule.

## 1.1 Motivating examples

The initial motivation of this series of papers lies in the striking interplay established in some cases between the computational complexity and the dynamical properties of automata networks. These two aspects are often measured in terms of periods of attractors or transient length and the computational complexity of various prediction or reachability problems respectively. The prediction problem consists in predicting the future state of an objective node, given an initial condition and has been widely studied for different classes of automata networks [25, 29, 26, 24] or cellular automata [42, 32, 41, 27]. The reachability problems generally asks whether a given input configuration will reach a given target configuration [5, 4], sometimes giving only partial information on the target configuration [17]. It has also been considered in a much generalized version as a benchmark for computational universality for arbitrary symbolic dynamical systems [12].

However, if we consider only these measurements, the link between computational complexity and dynamical complexity in a particular automata network family is not clear. In fact, different families exhibit various types of behavior both from a computational and from a dynamical standpoint. Let us consider three of them: threshold networks, algebraic networks and the outer-totalistic networks.

In the first family, all the nodes hold a binary state: 0 or 1. In addition, an integer  $\theta_v$  is assigned to each node representing its *threshold*. The dynamics of the network is defined locally by the sum of the states of its neighbors. If at least  $\theta_v$  neighbors of  $v$  are in state 1 the node  $v$  will change its internal state to 1. In any other case, the node will change its state to 0. A standard example of threshold networks are majority networks where  $\theta_v$  is set to half the size of the neighborhood. A seminal result [22, 31] shows that symmetric threshold networks (the underlying interaction graph is symmetric) cannot have periodic orbits of period more than 2, and that they have polynomially bounded transients; this implies the existence of a polynomial time algorithm to predict the future of a node from any given initial configuration [25], however the prediction problem can be P-complete on symmetric majority networks [41]. Here, the strong limitation on attractor periods does not totally exclude computational complexity. On the other hand, majority networks under partially asynchronous updates (precisely block-sequential update modes) were shown to have super-polynomial periodic orbits and a PSPACE-complete prediction problem [30, 9]. A similar result was obtained recently for conjunctive networks under a more general update mode called 'firing memory' [28].

The second family, the algebraic networks, are networks that have a linear global map and can be represented by a matrix. Thus, all orbits of the system are completely captures by the powers of the corresponding matrix. A notorious example is the case of the elementary 1D cellular automata rule 90 in which the local rule in each cell is simply the sum modulo 2 of the states of the left and the right neighbors. On one hand it is shown in [37] that the largest period  $\pi_N$  of a periodic orbits of this CA on a network of size  $N$  is exponential, precisely:  $\Pi_N \leq 2^{\frac{N-1}{2}} - 1$  for all  $N$  and  $\limsup_N \frac{\log \Pi_N}{N} = \frac{1}{2}$ , but the value of  $\Pi_N$  highly depends on the multiplicative number theoretic properties of  $N$ . On the other hand, since an orbit is determined by the powers of some matrix, the prediction problem can be solved by an efficient parallel algorithm (see for example [25] for an efficient algorithm for the prediction problem on disjunctive networks and [33] for more details on efficient parallel algorithms for the prefix sum problem). Here, the strongly limited computational complexity does not exclude long periods of attractors.

As a last example, the outer-totalistic networks are characterized by dynamics depending only in the state of the node and the sum of the states of the neighbors. A very famous example is the cellular automaton known as

Conway's *Game of Life*. In this two dimensional cellular automaton, each cell can be either dead or alive and the state of each cell depends on how many alive cells are nearby. If a cell is dead and has exactly 3 alive neighbors, or if it is alive and has 2 or 3 alive neighbors, then the cell is alive at the next step. In any other case, the cell is dead at the next step. In [15], this cellular automaton is shown to be intrinsically universal, *i.e.* able to closely simulate any other cellular automaton. It has consequences in terms of computational complexity but also dynamics [11, 23]. These two forms of complexity can be observed on periodic configurations, where the cellular automaton can be seen as a family of (finite) automata networks, and through hardness of the prediction problem and exponential periods of attractors for instance.

## 1.2 Our contributions

The previous examples show that focusing on a single aspect (like exponential periods of some orbits, or the hardness of a prediction problem) is not enough to accurately describe the complexity of families of automata networks. Moreover, complexity of different parameters or problems for a family can have a common root with many consequences in terms of complexity. Intrinsic universality, *i.e.* the ability to simulate arbitrary behaviors of automata networks, is such a common root. This notion has been successfully developed in the context of cellular automata [23, 11, 45, 43, 7, 38] and for other models like self-assembly tilings [16, 14, 40]. Although it appears implicitly in some results like in [20], the notion has never been explicitly ported to automata networks to our knowledge. In this paper, as our first main contribution, we explore this idea in depth: we develop a formalism of intrinsic simulation and universality for families of automata networks, and we study its implication for various notions of complexity, both of dynamical and computational nature. Our approach is not a priori limited to a small set of benchmark problems or properties: universality results can be used as a black box to then prove new corollaries on the complexity of other decision problems or other dynamical aspects.

We aim at making our approach general and modular, while giving concrete and relevant examples that were considered in literature. That is why, behind the main goals of the paper presented above, we carefully deal with many aspects of the formalism that are often left implicit in the literature or treated in a specific way for selected examples. A more detailed list of our contributions is as follows:

1. We define general notion of family of automata networks (Definition 4) that takes care of the size and complexity of representations.
2. As a running example we consider a set of concrete families (Definition 3) that capture many natural examples from the literature (Section 2.1) and will be at the heart of the companion papers.
3. We define a notion of intrinsic simulation between families of automata networks (Definition 7) and define two variants of intrinsic universality (Definition 13).
4. We study the theoretical implications of universality in the computational complexity of various problems (Corollary 1) as well as dynamical complexity (Theorem 15).
5. We show that, while universality implies hardness of all problems, there exist non-universal families which are hard for one problem but easy for another (Theorems 10 and 11). We also show that neither polynomially bounded periods nor polynomially bounded transients can discard a maximal complexity of the prediction problem alone, but both bounds together does (Theorem 12).
6. We show that the automata network family associated to an intrinsically universal of cellular automata lies between our two notions of intrinsic universality for automata networks (Theorems 17 and 18).

In the second paper of this series [46], we establish a general framework to make proofs based on gadget, suitable to prove intrinsic simulation and universality, even for families with symmetric networks which are prone to feedback problems. At the core of our approach is a concept of glueing of small unoriented networks, which permits to build a large network with a prescribed oriented flow of information through the dynamics (pseudo-orbits). This proof technique is applied in the third paper of the series [47], which deals with the effect of changing the update schedules with respect to intrinsic universality.

## 2 Automata networks and families

A directed *graph* is a pair  $G = (V, E)$  where  $V$  and  $E$  are finite sets satisfying  $E \subseteq V \times V$ . We will call  $V$  the set of *nodes* and the set  $E$  of *edges*. We call  $|V|$  the *order* of  $G$  and we usually identify this quantity by the letter  $n$ . Usually, as  $E$  and  $V$  are finite sets we will implicitly assume that there exists an ordering of the vertices in  $V$  from 0 to  $n - 1$ . Sometimes we will denote this set as  $[n]$ . If  $G = (V, E)$  and  $V' \subseteq V, E' \subseteq E$  we say that  $G'$  is a *subgraph* of  $G$ . When for every  $e = (u, v) \in E$  we have that  $(v, u) \in E$  we say that  $G$  is *symmetric*. From now on, we call every symmetric graph just a *graph* when the context is clear.

We call a graph  $P = (V, E)$  of the form  $V = \{v_1, \dots, v_n\}$   $E = \{(v_1 v_2), \dots, (v_{n-1}, v_n)\}$  a *directed path graph* or simply a *directed path*. When  $P$  is a symmetric path, we call  $P$  simply a *path*.

We often refer to a path by simply denoting its sequence of vertices  $\{v_1, \dots, v_n\}$ . We denote the *length* of a path by its number of edges. Whenever  $P = (V = \{v_1, \dots, v_n\}, E = \{(v_1 v_2), \dots, (v_{n-1}, v_n)\})$  is a path we call the graph in which we add the edge  $(v_n, v_1)$  a *cycle graph* or simply a *cycle* and we call it  $C$  where  $C = (V, E \cup \{(v_n, v_1)\})$ . Analogously, we distinguish the symmetric case from the directed case and we use the same nomenclature that we use for paths. In addition, a cycle is denoted usually by a sequence of nodes and its length is also given by the amount of edges (or vertices) in the cycle. Depending on the length of  $C$  we call it a  $k$ -cycle when  $k$  is its length.

A non-empty graph is called *connected* if any pair of two vertices  $u, v$  are linked by some path. Given any non-empty graph, a maximal connected subgraph is called a connected component. There is also a natural extension of the definition of paths, cycles and connectivity for directed graphs in the obvious way. We say a directed graph is *strongly connected* if there is a directed path between any two nodes. A strongly connected component of a directed graph  $G = (V, E)$  is a maximal strongly connected subgraph.

Given a (symmetric) graph  $G = (V, E)$  and two vertices  $u, v$  we say that  $u$  and  $v$  are neighbors if  $(u, v) \in E$ . Remark that abusing notations, an edge  $(u, v)$  is also denoted by  $uv$ . Let  $v \in V$ , we call  $N_G(v) = \{u \in V : uv \in E\}$  (or simply  $N(v)$  when the context is clear) the set of neighbors (or *neighborhood*) of  $v$  and  $\delta(G)_v = |N_G(v)|$  to the *degree* of  $v$ . Observe that if  $G' = (V', E')$  is a subgraph of  $G$  and  $v \in V'$ , we can also denote by  $N_{G'}(v)$  the set of its neighbors in  $G'$  and the degree of  $v$  in  $G'$  as  $\delta(G')_v = |N_{G'}(v)|$ . In addition, we define the *closed neighborhood* of  $v$  as the set  $N[v] = N(v) \cup \{v\}$  and we use the following notation  $\Delta(G) = \max_{v \in V} \delta_v$  for the *maximum degree* of  $G$ . Additionally, given  $v \in V$ , we will denote by  $E_v$  its set of *incident edges*, i.e.,  $E_v = \{e \in E : e = uv\}$ . We will use the letter  $n$  to denote the order of  $G$ , i.e.  $n = |V|$ . Also, if  $G$  is a graph whose sets of nodes and edges are not specified, we use the notation  $V(G)$  and  $E(G)$  for the set of vertices and the set of edges of  $G$  respectively. In the case of a directed graph  $G = (V, E)$  we define for a node  $v \in V$  the set of its *in-neighbors* by  $N^-(v) = \{u \in V : (u, v) \in E\}$  and its *out-neighbors* as  $N^+(v) = \{u \in V : (v, u) \in E\}$ . We have also in this context the indegree of  $v$  given by  $\delta^- = |N^-(v)|$  and its *outdegree* given by  $\delta^+ = |N^+(v)|$ .

During the most part of the text, and unless explicitly stated otherwise, every graph  $G$  will be assumed to be connected and undirected. We start by stating the following basic definitions, notations and properties that we will be using in the next sections. Recall that  $Q$  and  $V$  will denote finite sets representing the alphabet and the set of nodes respectively. We define  $\Sigma(Q)$  as the set of all possible permutations over alphabet  $Q$ . We call an *abstract automata network* any function  $F : Q^V \rightarrow Q^V$ . Note that  $F$  induces a dynamics in  $Q^V$  and thus we can see  $(Q^V, F)$  as dynamical system. In this regard, we recall some classical definitions. We call a *configuration* any element  $x \in Q^V$ . If  $S \subseteq V$  we define the restriction of a configuration  $x$  to  $V$  as the function  $x|_S \in Q^S$  such that  $(x|_S)_v = x_v$  for all  $v \in S$ . In particular, if  $S = \{v\}$ , we write  $x_v$ .

Given an initial configuration  $x \in Q^V$ , we define the *orbit* of  $x$  as the sequence  $\mathcal{O}(x) = (F^t(x))_{t \geq 0}$ . We define the set of *limit configurations* or *recurrent configurations* of  $F$  as  $L(F) = \bigcap_{t \geq 0} F^t(Q^V)$ . Observe that since  $Q$  is finite and  $F$  is deterministic, each orbit is *eventually periodic*, i.e. for each  $x \in Q^V$  there exist some  $\tau, p \in \mathbb{N}$  with  $p > 0$  such that  $F^{\tau+p}(x) = F^\tau(x)$  for all  $x \in Q^V$ . Note that if  $x$  is a limit configuration then its orbit is *periodic* (meaning  $\tau = 0$ ). In addition, any configuration  $x \in Q^V$  eventually reaches a limit configuration in finite time. We call that time the *transient time*, *transient length* or simply *transient* of the orbit induced by  $x$ . The maximum time that a configuration takes to reach a limit configuration is called the *transient* of  $F$ . We denote the set of orbits corresponding to periodic configurations as  $\text{Att}(F) = \{\mathcal{O}(x) : x \in L(F)\}$  and we call it the set of *attractors* of  $F$ . We define the *global period* or simply the *period* of  $\bar{x} \in \text{Att}(F)$  by  $p(\bar{x}) = \min\{p \in \mathbb{N} : \bar{x}(p) = \bar{x}(0)\}$ . If  $p(\bar{x}) = 1$  we say that  $\bar{x}$  is a *fixed point* and otherwise, we say that  $\bar{x}$  is a *limit cycle*.

**Remark 1.** Observe that in the context of this work the dynamics is defined by the application of function  $F$ . In the

literature this is described as a synchronous or a parallel update scheme. In all the next definitions and results we focus on this particular update scheme. We study the effect of asynchronism (i.e. different update schemes) on the third paper of this series [47].

Given a node  $v$ , its behavior  $x \mapsto F(x)_v$  might depend or not on another node  $u$ . This dependencies can be captured by a graph structure which plays an important role in the theory of automata networks (see [18] for a review of known results on this aspect). This motivates the following definitions.

**Definition 1.** Let  $F : Q^V \rightarrow Q^V$  be an abstract automata network and  $G = (V, E)$  a directed graph. We say  $G$  is a communication graph of  $F$  if for all  $v \in V$  there exist  $D \subseteq N_v^-$  and some function  $f_v : Q^D \rightarrow Q$  such that  $F(x)_v = f_v(x|_D)$ . The interaction graph of  $F$  is its minimal communication graph.

Note that by minimality, for any node  $v$  and any in-neighbor  $u$  of  $v$  in the interaction graph of some  $F$ , the next state at node  $v$  effectively depends on the actual state at node  $u$ . More precisely, there is some configuration  $c \in Q^V$  and some  $q \in Q$  with  $q \neq c_u$  such that  $F(c)_v \neq F(c')_v$  where  $c'$  is the configuration  $c$  where the state of node  $u$  is changed to  $q$ . This notion of effective dependency is sometimes taken as a definition of edges of the interaction graph.

From now on, for an abstract automata network  $F$  and some communication graph  $G$  of  $F$  we use the notation  $\mathcal{A} = (G, F)$ . In addition, by abuse of notation, we also call  $\mathcal{A}$  an abstract automata network. We define a set of automata networks or an *abstract family* of automata networks on some alphabet  $Q$  as a set  $\mathcal{F} \subseteq \bigcup_{n \in \mathbb{N}} \{F : Q^V \rightarrow Q^V : V \subseteq [n]\}$ .

Note that the latter definition provides a general framework of study as it allows us to analyze an automata network as an abstract dynamical system. However, as we are going to be working also with a computational complexity framework, it is necessary to be more precise in how we represent them. In this regard, one possible slant is to start defining an automata network from a communication graph. In fact, many commonly studied examples can be viewed as labeled graphs: for instance, linear networks are represented by a matrix (essentially an edge-labeled graph), and threshold networks can be seen as vertex and edge labeled graphs.

One of the main definition used all along this paper is that of *concrete symmetric automata network*. Roughly, they are symmetric labeled graph  $G$  (both on nodes and edges) that represent an automata network. They are *concrete* because the labeled graph is a natural concrete representation upon which we can formalize decision problems and develop a computational complexity analysis. They are *symmetric* in two ways: first their communication graph is symmetric, meaning that an influence of node  $u$  on node  $v$  implies an equivalent influence of node  $v$  on node  $u$ ; second, the behavior of a given node is blind to the ordering of its neighbors in the communication graph, and it can only differentiate its dependence on neighbors when the labels of corresponding edges differ.

A nice example of a CSAN is presented in Figure 2. The different labels represent *threshold* functions. For example  $\lambda_{\theta_1}$  correspond to a function that depends on the sum of the state of the neighbors of its corresponding vertex: if this sum is greater than  $\theta_1 = 3$  then, the function takes the value 1 and it takes the value 0 otherwise. Observe that these threshold functions can be represented as labels referencing its corresponding threshold value. In fact, this information can be represented as a number using  $\mathcal{O}(\log \Delta)$  bits where  $\Delta$  is the maximum degree of the graph. In addition, the label on the edges correspond to the identity function. As we will explain in the next section, in general, the size of the labels can be of size  $\mathcal{O}(\log \Delta)$  but in some known examples it can be constant.

A *multiset* over  $Q$  is a map  $m : Q \rightarrow \mathbb{N}$  (recall that  $0 \in \mathbb{N}$ ). A  $k$ -bounded multiset over  $Q$  is a map  $m : Q \rightarrow [k]$ , the set of such multisets is denoted  $[k]^Q$ . For instance a 2-bounded multiset is actually a set. Note that since  $Q$  is finite any multiset is actually a bounded multiset. To any (partial) configuration  $c \in Q^A$ , we associate the multiset  $m(c)$  which to any  $q \in Q$  associates its number of occurrences in  $c$ , i.e.

$$m(c) = q \mapsto |\{a \in A : c(a) = q\}|.$$

**Definition 2.** Given a symmetric graph  $G = (V, E)$ , a vertex label map  $\lambda : V \rightarrow (Q \times \mathbb{N}^Q \rightarrow Q)$  and a symmetric edge label map  $\rho : E \rightarrow (Q \rightarrow Q)$  (i.e.  $\rho(u, v) = \rho(v, u)$  for any  $(u, v) \in E$ ), we define the concrete symmetric automata network (CSAN)  $\mathcal{A} = (G, \lambda, \rho)$ . A family of concrete symmetric automata networks (CSAN family)  $\mathcal{F}$  is given by an alphabet  $Q$ , a set of local labeling constraints  $\mathcal{C} \subseteq \Lambda \times R$  where  $\Lambda = \{\phi : Q \times \mathbb{N}^Q \rightarrow Q\}$  is the set of possible vertex labels and  $R = 2^{\{\psi : Q \rightarrow Q\}}$  is the set of possible sets of neighboring edge labels. We say a CSAN  $(G, \lambda, \rho)$  belongs to  $\mathcal{F}$  if for any vertex  $v$  of  $G$  with incident edges  $E_v$  it holds  $(\lambda(v), \rho(E_v)) \in \mathcal{C}$ .

Note that the labeling constraints defining a CSAN family are local. In particular, the communication graph structure is a priori free. This aspect plays an important role in the second paper of this series [46] when building arbitrarily complex objects by composition of simple building blocks inside a CSAN family.

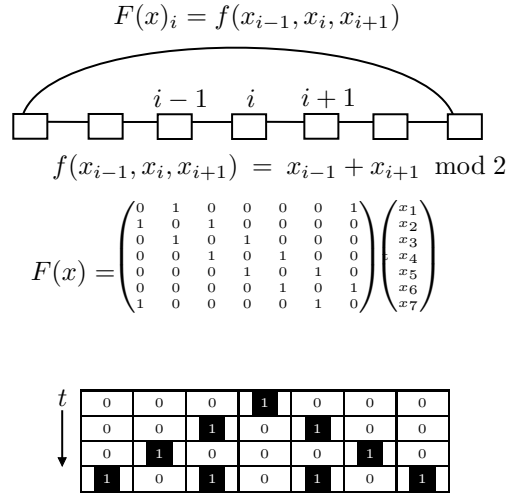


Figure 1: Representation and dynamics of Rule 90 for a cycle graph of 7 cells. From top to bottom: (1) interaction graph; (2) matrix representation and (3) dynamics.

Let us now define the abstract automata network associated to a CSAN, by describing the semantics of labels defined above. Intuitively, labels on edges are state modifiers, and labels on nodes give a map that describes how the node changes depending on the set of states appearing in the neighborhood, after application of state modifiers. We use the following notation: given  $\sigma : A \rightarrow (Q \rightarrow Q)$  a collection of state modifiers and  $x \in Q^A$  a partial configuration with  $A \subseteq V$ , we define  $x^\sigma = a \mapsto \sigma_a(x_a)$ .

**Definition 3.** Given a CSAN  $(G, \lambda, \rho)$ , its associated global map  $F : Q^V \rightarrow Q^V$  is defined as follows. For all node  $v \in V$  and for all  $x \in Q^V$ :

$$F(x)_v = \lambda_v(x_v, m((x|_{N(v)})^{\rho_v})),$$

with  $\rho_v : u \in N(v) \mapsto \rho(u, v)$ .

Note that if  $(G, \lambda, \rho)$  is a concrete automata network and  $F$  its global rule then,  $F$  is an abstract automata network with interaction graph included in  $G$ . Note also that for any vertex  $v$  and any configuration  $x$ , the multiset  $m(x|_{N(v)})$  is actually  $k$ -bounded where  $k$  is the degree of  $v$ .

## 2.1 Examples of CSAN networks

In this subsection, we provide some examples from the literature that can be modeled as CSAN networks. In each case we provide the elements that define the corresponding labeled graph representation of each family.

1. **Symmetric Linear networks.** When endowing the alphabet  $Q$  with a finite ring structure, we can consider maps  $F : Q^n \rightarrow Q^n$  defined by a  $n \times n$  matrix  $M = (M_{i,j})$  as  $F(x) = M \cdot x$  when seeing configurations as column vectors [49]. When  $M$  is symmetric, one can see  $F$  has the global map of a CSAN network defined as follows: the labeled graph  $(G, \lambda, \rho)$  is defined by non-zero entries of  $M$  and an edge between nodes  $i$  and  $j$  is labeled by the map  $q \mapsto M_{i,j}q$ , and, for each node  $i$ , the map  $\lambda_i$  is just the map computing the sum in the ring  $Q$  from a multiset, *i.e.* such that  $\lambda_i(x, m) = \sum_{q \in Q} m(q) \cdot q$ . We then have  $F(x)_i = \lambda_i(x_i, m((x|_{N(i)})^\rho)) = \sum_j M_{i,j}x_j$ . One of the most studied case is when  $Q$  is actually endowed with a field structure, in particular in the Boolean case where the choice of coefficient is unique and the automata network is entirely determined by the graph  $G$ . Note however, that considering non-Boolean finite fields makes a qualitative difference from the Boolean case for some properties (see for instance Proposition 3.5 and Corollary 4.3 of [8]). A very well studied example of a network in this family is the case of additive elementary cellular automata. In particular, the rule 90 in Wolfram notation, in which the new state of a cell is computed as the modulo 2 sum of its right and left neighbors. An example of its matrix representation for a small cycle graph of 7 cells is shown in Figure 1. In this case the matrix is defined over the field  $\mathbb{F}_2$ . In the same Figure, it is shown an example of its dynamics starting from a uniform random initial condition.

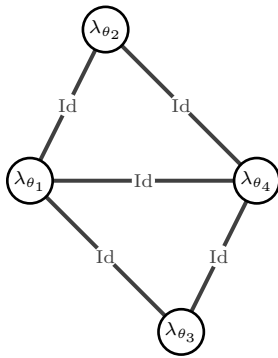


Figure 2: A threshold network in which  $\theta_1 = 2, \theta_2 = 1, \theta_3 = 1$  and  $\theta_4 = 2$ .

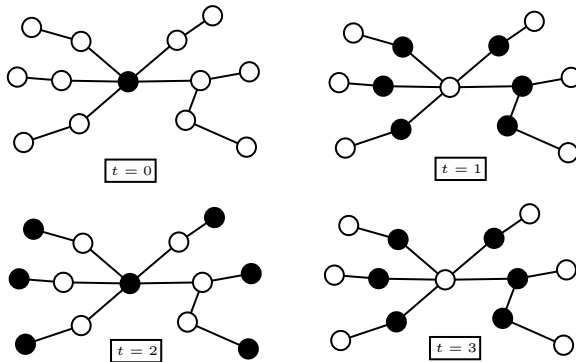


Figure 3: Dynamics of a threshold network where  $\theta_v = 1$  for every node  $v$  in the graph. Black nodes are in state 1 and white nodes are in state 0.

2. **Symmetric Threshold networks.** The threshold network family is a classical boolean network model that has been broadly studied both as a discrete dynamical system and also because of its computational properties [31, 22, 29, 25]. In this case, we have that  $Q = \{0, 1\}$ ,  $\rho = \{\text{Id}\}$  where Id is the identity function and the map

$$\text{at node } v \lambda_{\theta_v}(x, m) = \begin{cases} 1 & \text{if } m[1] - \theta_v \geq 0 \\ 0 & \text{otherwise,} \end{cases} \text{ for any multiset } m,$$

where  $\theta_v \in \mathbb{Z}$  is called the *threshold* associated to node  $v$ . An example of a threshold network represented as labeled graph is shown in Figure 2. In that example, the threshold values are chosen so that each node will change its state to 1 if and only if the strict majority of their neighbors are in state 1. Another example in which we exhibit the dynamics of a threshold network is the one Figure 3. In this example the threshold are all the same and equal to 1. In other words, each node will update its state to one if it has at least one neighbor in state 1. In the same Figure, it is shown a particular case in which the dynamics reaches an attractor of period 2.

3. **Symmetric Min/Max networks.** In this example, the local functions of each node in the network will compute the minimum or the maximum state value in the set of different states. Formally, let  $Q$  be a totally ordered set. Given a multiset  $m \in \mathbb{N}^Q$ , we denote by  $\min X = \min\{q \in Q : X(q) > 0\}$ . The family of *min-max automata networks* over  $Q$  is the set of CSAN  $(G, \lambda, \rho)$  such that for each edge  $e$ ,  $\rho_e$  is the identity map and, for each node  $v$ ,  $\lambda_v(q, X) = \max X$  or  $\lambda_v(q, X) = \min X$ . An interesting particular case is the case in which the set of states is just 0 and 1. In this case, the min-max automata networks are just the AND-OR networks, which have been broadly studied in the literature [28, 2]. More precisely, if  $Q = \{0, 1\}$  then,  $\lambda(x)_i = \bigwedge_{j \in N(i)} x_j$

or  $\lambda(x)_i = \bigvee_{j \in N(i)} x_j$ , for each node  $i \in V$ . In Figure 4 there is an example of an AND-OR network defined on a graph of 4 nodes.

4. **Symmetric Outer-totalistic Boolean automata networks.** In this case, the alphabet is binary and local function  $\lambda_v$  associated to each node in the network depends only the truncated sum of neighboring states, *i.e.* on the number of occurrences of each state counted up to some constant number. In addition the edge labels  $\rho$  are simply given by the identity function. An illustrative example is the famous Conway's Game of Life. In fact, in this case the next state of a cell depends only on its current state (dead or alive) and the amount of



black cells and white cells (dead or alive neighbors).

*Life-like rules* A classical example are the so-called life-like rules. These rules are defined for a binary alphabet where 1 represents 'alive' nodes and 0 dead ones, and the local rule is determined by two subsets  $B$  (for birth) and  $S$  (for survive) as follows: a dead node will change to state 1 if the sum of the states of its neighbors is in  $B$ , and an alive nodes stays alive if and only if the sum of neighboring states belongs to  $S$ . A notable example (that actually inspired the definition of this class) is Conway's Game of Life defined by  $B = \{3\}$  and  $S = \{2, 3\}$ .

*Interval rules.* Another natural class of examples are so-called interval rules defined by an interval  $[\alpha, \beta]$  where  $0 \leq \alpha \leq \beta$  and a cell will change to state 1 if the sum the states of its neighbors is a number that is at least  $\alpha$  and at most  $\beta$ . Observe that this case is similar to the latter family. In fact, the only difference is that for life-like rules, the transition rule depends on the state of each cell and the states of the neighbors and in the interval rules a cell depends only in the states of its neighbors. The communication graph of an interval rule with  $\alpha = 3$  and  $\beta = 4$  is shown in Figure 5. In addition, an example of a dynamics induced by an interval rule is shown in Figure 6. In the case shown in the figure, the interval is given by  $\alpha = 1$  and  $\beta = 2$ . In other words, a node will update its state to 1 if it has exactly one or two neighbors in state 1 and it will update its state to 0 otherwise.

5. **Reaction-difussion networks.** This family is similar to the case of Threshold networks. However, there is a non-trivial set of possible labels for the edges. In this case we have that  $Q = \alpha \cup \epsilon$  where  $\alpha = \{0, 1\}$  and  $\epsilon = \{2, \dots, q'\}$  and  $q' \geq 2$ . Roughly speaking,  $Q$  has reluctant states  $\{0\} \cup \epsilon$  and an active state 1. If a node reaches state 1 it will automatically go to the next state until it will reach  $q'$ . However, while the node goes from 2 to  $q'$  it will be considered as inactive for its neighbors. When a node  $v$  is in state 0 it needs at least  $\theta_v$  active neighbors to turn into 1. More precisely, we define these CSAN networks by setting  $\rho(e)$  to be the map

$$\begin{cases} 1 & \text{if } a = 1 \\ 0 & \text{otherwise} \end{cases} \text{ and } \lambda_{\theta_v}(x_v, m) = \begin{cases} 1 & \text{if } m[1] - \theta_v \geq 0 \wedge x_v = 0 \\ x_v + 1 & \text{if } x_v \neq 0 \wedge x_v \neq q' \\ 0 & \text{otherwise,} \end{cases} \quad \text{where } m \text{ is any multiset.}$$

An example of a reaction-diffusion dynamics is given in Figure 7. In this case, there is only one reluctant state ( $q' = 2$ ) and all the thresholds are set to 0 as same as in the example shown in Figure 3. In addition, observe that the graph is the same graph shown in Figure 3. However, as reaction-diffusion dynamics considers a reluctant state, the dynamics reaches a uniform fixed point contrary to the case of Figure 3 in which the dynamics reaches an attractor of period two, starting from the same initial condition.

### 3 Representing Automata Networks

As we are interested in measuring computational complexity of decision problems related to the dynamics of automata networks belonging to a particular family, their representation has to be specified precisely. We can always choose to represent automata networks through Boolean circuits. However, as we show in the first part of this section, families can have different natural representation which are closely related to their particular properties. Considering this fact, we introduce the notion of *standard representation* associated to a family: it can be any encoding of automata networks from the family provided we can efficiently obtain a circuit representation from it. Finally, we resume previous discussion on different representations for some particular families, showing how difficult it is to transform one particular representation into another one.

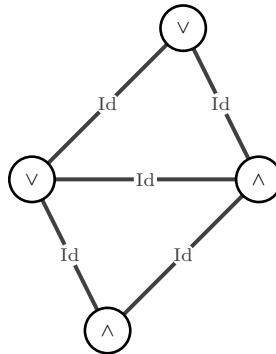


Figure 4: An AND-OR network.

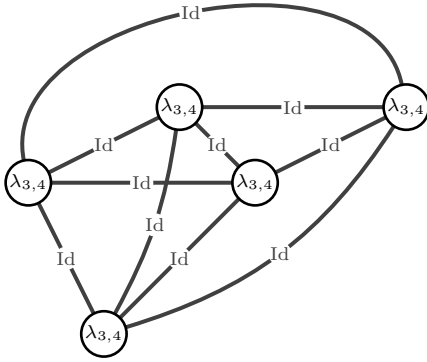


Figure 5: Interval rule network for  $\alpha = 3, \beta = 4$ .

### 3.1 Standard representations

We fix for any alphabet  $Q$  an injective map  $m_Q : Q \rightarrow \{0, 1\}^{k_Q}$  which we extend cell-wise for each  $n$  to  $m_Q : Q^n \rightarrow \{0, 1\}^{k_{Q^n}}$ . Given an abstract automata network  $F : Q^n \rightarrow Q^n$ , a circuit encoding of  $F$  is a Boolean circuit  $C : \{0, 1\}^{k_{Q^n}} \rightarrow \{0, 1\}^{k_{Q^n}}$  such that  $m_Q \circ F = C \circ m_Q$  on  $Q^n$ . We also fix a canonical way to represent circuits as words of  $\{0, 1\}^*$  (for instance given by a number of vertices, the list of gate type positioned at each vertex and the adjacency matrix of the graph of the circuit).

**Definition 4.** Let  $\mathcal{F}$  be a set of abstract automata network over alphabet  $Q$ . A standard representation  $\mathcal{F}^*$  for  $\mathcal{F}$  is a language  $L_{\mathcal{F}} \subseteq \{0, 1\}^*$  together with a **DLOGSPACE** algorithm such that:

- the algorithm transforms any  $w \in L_{\mathcal{F}}$  into the canonical representation of a circuit encoding  $C(w)$  that code an abstract automata network  $F_w \in \mathcal{F}$ ;
- for any  $F \in \mathcal{F}$  there is  $w \in L_{\mathcal{F}}$  with  $F = F_w$ .

The default general representations we will use are circuit representations, *i.e.* representations where  $w \in L_{\mathcal{F}}$  is just a canonical representation of a circuit. In this case the **DLOGSPACE** algorithm is trivial (the identity map). However, we sometimes want to work with more concrete and natural representations for some families of networks: in such a case, the above definition allows any kind of coding as soon as it is easy to deduce the canonical circuit representation from it.

### 3.2 Example of standard representations of some particular families

Observe that communication graph is often an essential piece of information for describing an automata network, however, this information is usually not enough. In this section three examples of canonical types of families are discussed: bounded degree networks, CSAN and algebraic families. They all have the property that a complete description of an automata network can be done in a size comparable to the communication graph (more precisely, polynomial in the number of nodes), *i.e.* much less than the set of all possible configurations.

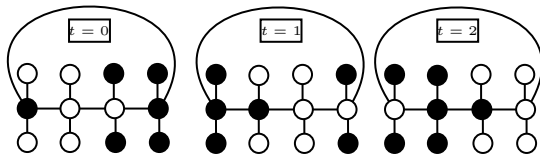


Figure 6: Dynamics of the interval rule  $[1, 2]$ . Black cells are in state 1 and white cells are in state 0.

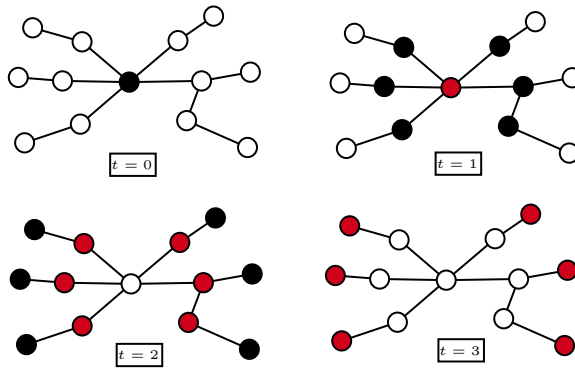


Figure 7: An example of a dynamics of a reaction-diffusion network with only one reluctant state and  $\theta_v = 1$  for any node in the network. Nodes in black are nodes in state 1, nodes in red are in reluctant state and nodes in white are in state 0.

**The CSAN case** A CSAN family is a collection of labeled graphs and thus is naturally represented as a graph  $G$  together with some representations of local functions (i.e.  $\lambda$  and  $\rho$ ). At each node  $v \in V$  the local function  $\lambda(v)$  will only be applied to pairs made of a state and a  $k$ -bounded multiset of states where  $k$  is the degree of  $v$ . In any case, it holds  $k \leq |V| = n$  so it is sufficient to consider only  $n$ -bounded multisets in order to completely specify the global map of the CSAN (Definition 3). For a fixed alphabet  $Q$ , there are  $(n+1)^{|Q|}$  distinct  $n$ -bounded multisets so any  $\lambda(v)$  can be described via a table of states of  $Q$  of size polynomial in the graph  $G$ . There are only finitely many possible  $\rho$  maps and we represent them by an arbitrary numbering. From the graph  $G$ , the table describing  $\lambda(v)$  and the  $\rho$  labels of adjacent edges, it is not difficult to produce in **DLOGSPACE** a circuit that computes the transition map  $F_v$  of node  $v$  following Definition 3. We therefore have a standard representation for CSAN families where the encoding of an automata network is made of the encoding of  $G$ , the encoding of  $\lambda(v)$  for each node  $v$  and the encoding of  $\rho_e$  for each edge  $e$ . This encoding is of size polynomial in the number of nodes.

**The case of bounded degree communication graphs** Let us fix some positive constant  $\Delta$ . It is natural to consider the family of automata networks whose interaction graph has a maximum degree bounded by  $\Delta$ . We associate to this family the following representation: an automata network  $F$  is given as a pair  $(G, (\tau_v)_{v \in V(G)})$  where  $G$  is a communication graph of  $F$  of maximum degree at most  $\Delta$  and  $(\tau_v)_{v \in V(G)}$  is the list for all nodes of  $G$  of its local transition map  $F_v$  of the form  $Q^d \rightarrow Q$  for  $d \leq \Delta$  and represented as a plain transition table of size  $|Q|^d \log(|Q|)$ .

**Remark 2.** *Given any CSAN family, there is a **DLOGSPACE** algorithm that transforms a bounded degree representation of an automata network of the family into a CSAN representation: indeed in this case all local maps are bounded objects, so it is just a matter of making a bounded computation for each node.*

**The algebraic case** When endowing the alphabet  $Q$  with a finite field structure, the set of configurations  $Q^n$  is a vector space and one can consider automata networks that are actually linear maps. In this case the natural representation is a  $n \times n$  matrix. It is clearly a standard representation in the above sense since circuit encodings can be easily computed from the matrix. Moreover, as in the CSAN case, when a linear automata network is given as a bounded degree representation, it is easy to recover a matrix in **DLOGSPACE**.

More generally, we can consider matrix representations without field structure on the alphabet. An interesting case is that of Boolean matrices:  $Q = \{0, 1\}$  is endowed with the standard Boolean algebra structure with operations  $\vee, \wedge$  and matrix multiplication is defined by:

$$(AB)_{i,j} = \bigvee_k A_{i,k} \wedge B_{k,j}.$$

They are a standard representation of disjunctive networks (and by switching the role of 0 and 1 conjunctive networks), i.e. networks  $F$  over alphabet  $\{0, 1\}$  whose local maps are of the form  $F_i(x) = \bigvee_{k \in N(i)} x_k$  (respectively  $F_i(x) = \bigwedge_{k \in N(i)} x_k$ ). When their dependency graph is symmetric, disjunctive networks (resp. conjunctive networks) are a particular case of CSAN networks for which  $\rho_v$  maps are the identity and  $\lambda(v)$  are just max (resp. min) maps. For disjunctive networks (resp. conjunctive networks) the CSAN representation and the matrix representation are **DLOGSPACE** equivalent.

### 3.3 Computing interaction graphs from representations

One of the key differences between all the representations presented so far is in the information they give about the interaction graph of an automata network. For instance, it is straightforward to deduce the interaction graph of a linear network from its matrix representation in **DLOGSPACE**: the non-zero entries of the matrix gives the edges of the interaction graph. The situation doesn't change much if the linear network is given by a circuit representation: it is sufficient to evaluate the circuit on the  $n$  input configurations that form a base of the vector space  $Q^n$  to completely know the matrix of the linear network.

At the other extreme, one can see that it is NP-hard to decide whether a given edge belongs to the interaction graph of an automata network given by a circuit representation: indeed, one can build in **DLOGSPACE** from any SAT formula  $\phi$  with  $n$  variables a circuit representation of an automata network  $F : \{0, 1\}^{n+1} \rightarrow \{0, 1\}^{n+1}$  with

$$F(x)_1 = \begin{cases} x_{n+1} & \text{if } \phi(x_1, \dots, x_n) \text{ is true,} \\ 0 & \text{else.} \end{cases}$$

This  $F$  is such that node 1 depends on node  $n + 1$  if and only if  $\phi$  is satisfiable.

For automata networks with communication graphs of degree at most  $\Delta$ , there is a polynomial time algorithm to compute the interaction graph from a circuit representation: for each node  $v$ , try all the possible subsets  $S$  of nodes of size at most  $\Delta$  and find the largest one such that the following map

$$x \in Q^S \mapsto F_v(\phi(x))$$

effectively depends on each node of  $S$ , where  $\phi(x)_w$  is  $x_w$  if  $w \in S$  and some arbitrary fixed state  $q \in Q$  else. Note also, that we can compute a bounded degree representation in polynomial time with the same idea.

In the CSAN case, the situation is ambivalent. On one hand, the interaction graph can be computed in polynomial time (in the number of nodes) from a CSAN representation because for any given node  $v$  there is only polynomially many possible multiset of the form  $m((x|_{N(v)})^\rho)$  that can appear in the neighborhood of  $v$  and, for each neighbor  $v'$  of  $v$ , we can compute (in polynomial time) the set of pairs of such multisets that can be realized by changing just the state of  $v'$ . This allows to determine whether  $v$  depends on  $v'$  by verifying whether any such pair can change the state of  $v$  through the local map  $\lambda_v$ . The dependence of  $v$  on itself is also easy to check once the set of possible multisets is computed.

On the other hand, a polynomial time algorithm to compute the interaction graph from a circuit representation would give a polynomial algorithm solving Unambiguous-SAT (which is very unlikely following Valiant-Vazirani theorem [52]). Indeed, any "dirac" map  $\delta : \{0, 1\}^n \rightarrow \{0, 1\}$  with  $\delta(x) = 1$  if and only if  $x_1 \cdots x_n = b_1 \cdots b_n$  can be seen as the local map of a CSAN network because it can be written as  $\gamma(\{\rho_i(x_i) : 1 \leq i \leq n\})$  where  $\rho_i(x_i) = x_i$  if  $b_i = 1$  and  $\neg x_i$  else, and  $\gamma$  is the map  $[2]^{\{0,1\}} \rightarrow \{0, 1\}$

$$S \subseteq Q \mapsto \begin{cases} 1 & \text{if } S = \{1\} \\ 0 & \text{else.} \end{cases}$$

A constant map can also be seen as the local map of some CSAN network. Therefore, given a Boolean formula  $\phi$  with the promise that is at has at most one satisfying assignment, one can easily compute the circuit representation of some CSAN network which has some edge in its interaction graph if and only if  $\phi$  is satisfiable: indeed, the construction of  $F$  above from a SAT formula always produce a CSAN given the promise on  $\phi$ .

It follows from the discussion above that a polynomial time algorithm to compute a CSAN representation of a CSAN represented by circuit would give a polynomial time algorithm to solve Unambiguous-SAT.

The following table synthesizes the computational hardness of representation conversions. It shall be read as follows: given a family  $(\mathcal{F}, \mathcal{F}^*)$  listed horizontally and a family  $(\mathcal{H}, \mathcal{H}^*)$  listed vertically, the corresponding entry in the table indicates the complexity of the problem of transforming  $w \in L_{\mathcal{F}}$  with the promise that  $F_w \in \mathcal{F} \cap \mathcal{H}$  into  $w' \in L_{\mathcal{H}}$  such that  $F_w = H_{w'}$ .

output \ input	circuit	CSAN	$\Delta$ -bounded degree	matrix
circuit	trivial	<b>DLOGSPACE</b>	<b>DLOGSPACE</b>	<b>DLOGSPACE</b>
CSAN	USAT-hard	trivial	<b>DLOGSPACE</b>	<b>DLOGSPACE</b>
$\Delta$ -bounded degree	PTIME	PTIME	trivial	<b>DLOGSPACE</b>
matrix	PTIME	<b>DLOGSPACE</b>	<b>DLOGSPACE</b>	trivial

USAT-hard means that any PTIME algorithm would imply a PTIME algorithm for Unambiguous-SAT.

## 4 Simulation and universality

In this section we introduce a key tool used in this paper: simulations. The goal is to easily prove computational or dynamical complexity of some family of automata networks by showing it can simulate some well-known reference family where the complexity analysis is already established. It can be thought as a complexity or dynamical reduction. Simulations of various kinds are often implicitly used in proofs of dynamical or computational hardness. We are going instead to explicitly define a notion of simulation and establish hardness results as corollaries of simulation results later in the paper. To be more precise, we will first define a notion of simulation between individual automata networks, and then extend it to a notion of simulation between families. This latter notion, which is the one we are really interested in requires more care if we want to use it as a notion of reduction for computational complexity. We introduce all the useful concepts progressively in the next subsections.

### 4.1 Simulation between individual automata networks

At the core of our formalism is the following definition of simulation where an automata network  $F$  is simulated by an automata network  $G$  with a constant time slowdown and using blocks of nodes in  $G$  to represent nodes in  $F$ . Our definition is rather strict and requires in particular an injective encoding of configurations of  $F$  into configurations of  $G$ . We are not aware of a published work with this exact same formal definition, but close variants certainly exist and it is a direct adaptation to finite automata networks of a classical definition of simulation for cellular automata [11].

**Definition 5.** Let  $F : Q_F^{V_F} \rightarrow Q_F^{V_F}$  and  $G : Q_G^{V_G} \rightarrow Q_G^{V_G}$  be abstract automata networks. A block embedding of  $Q_F^{V_F}$  into  $Q_G^{V_G}$  is a collection of blocks  $D_i \subseteq V_G$  for each  $i \in V_F$  which forms a partition of  $V_G$  together with a collection of patterns  $p_{i,q} \in Q_G^{D_i}$  for each  $i \in V_F$  and each  $q \in Q_F$  such that  $p_{i,q} = p_{i,q'}$  implies  $q = q'$ . This defines an injective map  $\phi : Q_F^{V_F} \rightarrow Q_G^{V_G}$  by  $\phi(x)_{D_i} = p_{i,x_i}$  for each  $i \in V_F$ . We say that  $G$  simulates  $F$  via block embedding  $\phi$  if there is a time constant  $T$  such that the following holds on  $Q_F^{V_F}$ :

$$\phi \circ F = G^T \circ \phi.$$

See Figure 8 for a scheme of block simulation. In the following, when useful we represent a block embedding as the list of blocks together with the list of patterns. The size of this representation is linear in the number of nodes (for fixed alphabet).

**Remark 3.** It is convenient in many concrete cases to define a block embedding through blocks  $D_i$  that are disjoint but do not cover  $V_G$  and add a context block  $C$  disjoint from the  $D_i$  that completes the covering of  $V_G$ . In this variant a block embedding of  $Q_F^{V_F}$  into  $Q_G^{V_G}$  is given by patterns  $p_{i,q}$  and a constant context pattern  $p_C \in Q_G^C$  which define an injective map  $\phi : Q_F^{V_F} \rightarrow Q_G^{V_G}$  by  $\phi(x)_{D_i} = p_{i,x_i}$  for each  $i \in V_F$  and  $\phi(x)_C = p_C$ . This variant is actually just a particular instance of Definition 5 because we can include  $C$  in an arbitrary block ( $D_i \leftarrow D_i \cup C$ ) and define the block embedding as in Definition 5.

Another natural particular case of Definition 5 corresponding to localized information is when in each block  $D_i$ , there is a special node  $v_i \in D_i$  such that the map  $q \mapsto p_{i,q}(v_i)$  is injective. It is only possible when  $Q_G$  is larger than  $Q_F$ , but it will be the case in several examples of Boolean automata networks below. Interestingly, this local coding phenomena is forced when some automata network  $G$  simulates some Boolean automata network  $F$ : indeed, in any block  $D_i$  of  $G$  at least one node  $v_i$  must change between patterns  $p_{i,0}$  and  $p_{i,1}$ , but the map  $x \in \{0,1\} \mapsto p_{i,x}$  being injective, it means that  $x \mapsto p_{i,x}(v_i)$  is injective too.

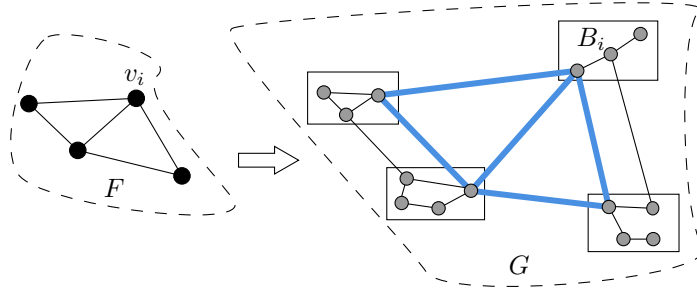


Figure 8: Scheme of one-to-one block simulation. In this case, network  $F$  is simulated by  $G$ . Each node in  $F$  is assigned to a block in  $G$  and state coding is injective. Observe that blocks are connected (one edge in the original graph may be represented by a path in the communication graph of  $G$ ) according to connections between nodes in the original network  $F$ . These connections are represented by blue lines.

**Remark 4.** The simulation relation of Definition 5 is a pre-order on automata networks.

The orbit graph  $G_F$  associated to network  $F$  with nodes  $V$  and alphabet  $Q$  is the directed graph with vertices  $Q^V$  and an edge from  $x$  to  $F(x)$  for each  $x \in Q^V$ . We also denote  $G_F^t = G_{F^t}$ .

**Lemma 6.** If  $G$  simulates  $F$  via block embedding with time constant  $T$  then the orbit graph  $G_F$  of  $F$  is a subgraph of  $G_G^T$ . In particular if  $F$  has an orbit with transient of length  $t$  and period of length  $p$ , then  $G$  has an orbit with transient of length  $Tt$  and period  $Tp$ .

*Proof.* The embedding of  $G_F$  inside  $G_G^T$  is realized by definition by the block embedding of the simulation. The consequence on the length of periods and transients comes from the fact that the embedding  $\phi$  verifies:  $x$  is in a periodic orbit if and only if  $\phi(x)$  is in a periodic orbit.  $\square$

## 4.2 Simulation between automata network families

From now on, a family of automata networks will be given as a pair  $(\mathcal{F}, \mathcal{F}^*)$  where  $\mathcal{F}$  is the set of abstract automata networks and  $\mathcal{F}^*$  a standard representation. We can now present our notion of simulation between families: a family  $\mathcal{A}$  can simulate another family  $\mathcal{B}$  if we are able to *effectively* construct for any  $B \in \mathcal{B}$  some automata network  $A \in \mathcal{A}$  that is able to simulate  $B$  in the sense of Definition 5. More precisely, we ask on one hand that the automata network which performs the simulation do this task in reasonable time and reasonable space in the *size of the simulated automata network*, and, on the other hand, that the construction of the simulator is efficient in the *size of the representation of the simulated one*.

**Definition 7.** Let  $(\mathcal{F}, \mathcal{F}^*)$  and  $(\mathcal{H}, \mathcal{H}^*)$  be two families with standard representations on alphabets  $Q_F$  and  $Q_H$  respectively. Let  $T, S : \mathbb{N} \rightarrow \mathbb{N}$  be two functions. We say that  $\mathcal{F}^*$  simulates  $\mathcal{H}^*$  in time  $T$  and space  $S$  if there exists a **DLOGSPACE** Turing machine  $M$  such that for each  $w \in L_{\mathcal{H}}$  representing some automata network  $H_w \in \mathcal{H} : Q_H^n \rightarrow Q_H^n$ , the machine outputs the following:

- $w' \in L_{\mathcal{F}}$  with  $F_{w'} : Q_F^{n_F} \rightarrow Q_F^{n_F}$ ,
- $T(n)$ ,
- a representation of a block embedding  $\phi : Q_F^{n_F} \rightarrow Q_H^n$ ,

such that  $n_F = S(n)$  and  $F_{w'}$  simulates  $H_w$  in time  $T = T(n)$  under block embedding  $\phi$ .

From now on, whenever  $\mathcal{F}^*$  simulates  $\mathcal{H}^*$  in time  $T$  and space  $S$  we write  $\mathcal{H}^* \preceq_{S,T}^T \mathcal{F}^*$ . In the above definition, the map  $T(n)$  represents the temporal rescaling factor for a simulated network of size  $n$ . The spatial rescaling factor is  $S(n)/n$ . In the sequel we will mostly consider two cases: when the spatio-temporal rescaling factors are polynomial in  $n$ , and when they are constant.

**Remark 5.** Note that both  $T$  and  $S$  maps must be **DLOGSPACE** computable from this definition. Moreover, the simulation relation between families is transitive because the class **DLOGSPACE** is closed under composition and simulation between individual automata networks is also transitive. When composing simulations time and space maps  $S$  and  $T$  get composed.

### 4.3 Decision problems and automata network dynamics

Studying the complexity of decision problems related to the dynamics of some discrete dynamical system is a very well known and interesting approach for measuring the complexity of the dynamics. In this section we introduce three variants of a classical decision problem that is closely related to the dynamical behavior of automata networks: the prediction problem. This problem consists in predicting the state of one node of the network at a given time. We study short term and long term versions of the problem depending on the way the time step is given in input. In addition, we explore a variant in which we ask if some node has eventually changed without specifying any time step, but only a constant observation time rate  $\tau$ . In other words, we check the system for any change on the state of a particular node every multiple of  $\tau$  time steps. The main point of this subsection is to show that these problems are coherent with our simulation definition in the sense that if some family of automata networks  $(\mathcal{F}_2, \mathcal{F}_2^*)$  simulates  $(\mathcal{F}_1, \mathcal{F}_1^*)$  then, if some of the latter problem is hard for  $\mathcal{F}_1$  it will also be hard for  $\mathcal{F}_2$ . We will precise this result in the following lines.

Let  $(\mathcal{F}, \mathcal{F}^*)$  an automata network family and let  $L \in \{0, 1\}^* \times \{0, 1\}^*$  be a parametrized language. We say that  $L$  is parametrized by  $\mathcal{F}$  if  $L$  has  $\mathcal{F}^*$  encoded as parameter. We note  $L_{\mathcal{F}} \in \{0, 1\}^*$  as the language resulting on fixing  $\mathcal{F}^*$  as a constant.

In particular, we are interested in studying prediction problems. We start by defining two variants of this well-known decision problem:

**Problem** (Unary Prediction (U-PRED)).

**Parameters:** *alphabet  $Q$ , a standard representation  $\mathcal{F}^*$  of an automata network family  $\mathcal{F}$*

**Input:**

1. a word  $w_F \in \mathcal{F}^*$  representing an automata network  $F : Q^n \rightarrow Q^n$  on alphabet  $Q$ , with  $F \in \mathcal{F}$ ,
2. a node  $v \in V(F) = [n]$ ,
3. an initial condition  $x \in Q^V$ ,
4. a state  $q \in Q$ ,
5. a natural number  $t$  represented in unary.

**Question:**  $F^t(x)_v = q$ ?

**Problem** (Binary Prediction (B-PRED)).

**Parameters:** *alphabet  $Q$ , a standard representation  $\mathcal{F}^*$  of an automata network family  $\mathcal{F}$*

**Input:**

1. a word  $w_F \in \mathcal{F}^*$  representing an automata network  $F : Q^n \rightarrow Q^n$  on alphabet  $Q$ , with  $F \in \mathcal{F}$ ,
2. a node  $v \in V(F) = [n]$ ,
3. an initial condition  $x \in Q^V$ ,
4. a state  $q \in Q$ ,
5. a natural number  $t$  represented in binary  $t \in \{0, 1\}^*$ .

**Question:**  $F^t(x)_v = q$ ?

Note that two problems are essentially the same, the only difference is the representation of time  $t$  that we call the *observation time*. We will also call node  $v$  the objective node. Roughly, as it happens with other decision problems, such as integer factorization, the representation of observation time will have an impact on the computation complexity of prediction problem. When the context is clear we will refer to both problems simply as PRED. In order to precise the latter observation we present now some general complexity results concerning PRED.

**Proposition 1.** *Let  $\mathcal{F}$  be a concrete automata network family. The following statements hold:*

1.  $U\text{-PRED}_{\mathcal{F}} \in P$
2.  $B\text{-PRED}_{\mathcal{F}} \in PSPACE$

Finally, we show that latter problem is coherent with our definition of simulation, in the sense that we can preserve the complexity of PRED. Note that this give us a powerful tool in order to classify concrete automata rules according to the complexity of latter decision problem.

**Lemma 8.** *Let  $(\mathcal{F}, \mathcal{F}^*)$  and  $(\mathcal{H}, \mathcal{H}^*)$  be two automata network families. Let  $T, S : \mathbb{N} \rightarrow \mathbb{N}$  be two polynomial functions such that  $\mathcal{H}^* \preceq_S^T \mathcal{F}^*$  then,  $PRED_{\mathcal{H}^*} \leq_L^T PRED_{\mathcal{F}^*}^{-1}$  where PRED denotes either U-PRED or B-PRED*

*Proof.* Let  $(w_H, v, x, q, t)$  be an instance of  $PRED_{\mathcal{H}^*}$ . By definition of simulation, there exists a **DLOGSPACE** algorithm which takes  $w_H$  and produces a word  $w_F \in L_{\mathcal{F}}$  with  $F : Q^{n_F} \rightarrow Q^{n_F}$  and a block representation  $\phi : Q^{n_F} \rightarrow Q^n$  such that  $n_F = S(n)$  and  $F$  simulates  $H$  in time  $T(n)$  under block embedding  $\phi$ . Particularly, there exists a partition of blocks  $D_v \subseteq V(F) = [n_F]$  for each  $v \in V(H) = [n]$  and a collection of injective patterns, i.e. patterns  $p_{i,q} \in Q_F^{D_i}$  such that  $p_{i,q} = p_{i,q'} \implies q = q'$ . In addition, we have  $\phi \circ H = F^T \circ \phi$ . Let us define the configuration  $y \in Q_F^{n_F}$  as  $y_{D_i} = p_{i,x_i}$ , i.e.,  $\phi(x)_{D_i} = y_{D_i}$ . Note that  $y$  is well-defined as the block map is injective. In addition, let us choose an arbitrary vertex  $v' \in D_v$  and an arbitrary  $q' \in Q_F$  and let us consider now the instance of  $PRED_{\mathcal{F}^*}$  given by  $(w_F, v', y, t \times T)$ . Note that for each  $v' \in D_v$  the transformation  $(w_H, v, x, q, t) \rightarrow (w_F, v', y, q', t \times T)$  can be done in **DLOGSPACE**( $|w_H|$ ) because we can read the representation of  $\phi$  for each block  $p_{i,x_i}$  and then output the configuration  $y$ . We claim that there exists a **DLOGSPACE**( $|w_H|$ ) algorithm that decides if  $(w_H, v, x, t) \in L_{PRED_{\mathcal{H}^*}}$  with oracle calls to  $PRED_{\mathcal{F}^*}$ . More precisely, as a consequence of the injectivity of block embedding, it is sufficient to runs oracle calls of  $PRED_{\mathcal{F}^*}$  for  $(w_F, v', q', y, t \times T)$  for a set of pairs  $v' \in D_v$  and  $q' \in Q_F$  of size at most  $|Q|$  in order to determine which pattern  $p_{v,q}$  verifies  $F^{t \times T}(y)_{D_v} = p_{v,q}$ . Finally, all of this can be done in **DLOGSPACE** as  $n_F = S(n) = n^{\mathcal{O}(1)}$  and  $T = n^{\mathcal{O}(1)}$  and thus, a polynomial amount of calls to each oracle is needed.  $\square$

Finally, we would like to study the case in which the observation time is not unique and ask whether the state of some node eventually changes. However, in order to preserve complexity properties under simulation, we still need to have some sort of restriction on observation times. This will allow us to avoid giving misleading answers when the simulating network is performing one step of simulation: indeed, it could take several time steps for the simulating network in order to represent one step of the dynamics of the simulated network, so some state change could happen in the intermediate steps while the simulated dynamics involve no state change. In order to manage this sort of time dilation phenomenon between simulating and simulated systems, we introduce the following decision problem.

**Problem** (Prediction change  $PRED\text{-CHG}_{\mathcal{F}^*}$ ).

**Parameters:** *alphabet  $Q$ , a standard representation  $\mathcal{F}^*$  of an automata network family  $\mathcal{F}$*

**Input:**

1. a word  $w_F \in \mathcal{F}^*$  representing an automata network  $F : Q^n \rightarrow Q^n$  on alphabet  $Q$ , with  $F \in \mathcal{F}$ ,
2. a node  $v \in V(G)$ ,
3. an initial condition  $x \in Q^V$ ,
4. a time gap  $k \in \mathbb{N}$  in unary.

**Question:**  $\exists t \in \mathbb{N} : F^{kt}(x)_v \neq x_v$

As we did with previous versions of prediction problem, we introduce a general complexity result and then, we show computation complexity is consistent under simulation.

**Proposition 2.** *Let  $(\mathcal{F}, \mathcal{F}^*)$  be a automata network family.  $PRED\text{-CHG}_{\mathcal{F}} \in PSPACE$ .*

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<sup>1</sup>Here we denote  $\leq_L^T$  as a **DLOGSPACE** Turing reduction. The capital letter ‘‘T’’ stands for *Turing reduction* and it is not related to the simulation time function which is also denoted by T.



The injectivity of block encodings in our definition of simulation is essential for the following lemma as it guaranties that a state change in the simulating network always represent a state change in the simulated network at the corresponding time steps.

**Lemma 9.** *Let  $(\mathcal{F}, \mathcal{F}^*)$  and  $(\mathcal{H}, \mathcal{H}^*)$  be two automata network families and  $T, S : \mathbb{N} \rightarrow \mathbb{N}$  two polynomial functions such that  $\mathcal{H}^* \preceq_S^T \mathcal{F}^*$  then,  $\text{PRED-CHG}_{\mathcal{H}^*} \leq_L^T \text{PRED-CHG}_{\mathcal{F}^*}$ .*

*Proof.* Proof is analogous to short term prediction case. Let  $(w_H, v, x, k)$  be an instance of  $\text{PRED-CHG}_{\mathcal{H}^*}$ . Again, by the definition of simulation, there exists a **DLOGSPACE** algorithm which takes  $w_H$  and produces a word  $w_F \in L_{\mathcal{F}}$  with  $F : Q^{n_F} \rightarrow Q^{n_F}$  and a block representation  $\phi : Q^{n_F} \rightarrow Q^n$  such that  $n_F = S(n)$  and  $F$  simulates  $H$  in time  $T(n)$  under block embedding  $\phi$ . The latter statements means, particularly, that there exists a partition of blocks  $D_v \subseteq V(F) = [n_F]$  for each  $v \in V(H) = [n]$  and a collection of injective patterns, i.e. patterns  $p_{i,q} \in Q_F^{D_i}$  such that  $p_{i,q} = p_{i,q'} \implies q = q'$  and also that  $\phi \circ H = F^{T(n)} \circ \phi$ . Let us define the configuration  $y \in Q_F^{n_F}$  as  $y_{D_i} = p_{i,x_i}$ , i.e.,  $\phi(x)_{D_i} = y_{D_i}$ . Note, again, that  $y$  is well-defined as the block map is injective. Now we proceed in using the same approach than before: for each  $v' \in D_v$  we can produce an instance  $(w_F, v', y, kT(n))$  of  $\text{PRED-CHG}_{\mathcal{F}^*}$ . There exists a **DLOGSPACE** machine which produces  $(w_F, v', y, kT(n))$  for each  $v' \in D_v$  and calls for an oracle solving  $\text{PRED-CHG}_{\mathcal{F}^*}(w_F, v', y, kT(n))$  and outputs 1 if there is at least one YES-instance for some  $v'$ . By definition of simulation and injectivity of block embedding function we have that this algorithm outputs 1 if and only if  $(w_H, v, x, k) \in \text{PRED-CHG}_{\mathcal{H}^*}$ .  $\square$

To end this subsection, let us show that problems  $\text{PRED-CHG}$  and  $\text{B-PRED}$  are actually orthogonal: depending of the family of automata networks considered, one can be harder than the other and reciprocally.

**Theorem 10.** *There exists a family with circuit representation  $(\mathcal{F}, \mathcal{F}^*)$  such that  $\text{B-PRED}_{\mathcal{F}}$  is solvable in polynomial time while  $\text{PRED-CHG}_{\mathcal{F}}$  is NP-hard. Conversely, there exists a family with circuit representation  $(\mathcal{G}, \mathcal{G}^*)$  such that  $\text{B-PRED}_{\mathcal{G}}$  is PSPACE-complete while  $\text{PRED-CHG}_{\mathcal{G}}$  is solvable in polynomial time.*

*Proof.* Given a SAT formula  $\phi$  with  $n$  variables, let us define the automata network  $F_\phi$  on  $\{0, 1\}^{n+1}$  which interprets any configuration as a pair  $(b, v) \in \{0, 1\} \times \{0, 1\}^n$  where  $b$  is the state of node 1 and  $v$  is both a number represented in base 2 and a valuation for  $\phi$  and does the following:

$$F(b, i) = \begin{cases} (1, i + 1 \bmod 2^n) & \text{if } \phi \text{ is true on valuation } v, \\ (0, i + 1 \bmod 2^n) & \text{else.} \end{cases}$$

A circuit representation of size polynomial in  $n$  can be computed in **DLOGSPACE** from  $\phi$  and we define  $(\mathcal{F}, \mathcal{F}^*)$  as the family obtained by considering all  $F_\phi$  for all SAT formulas  $\phi$ . First,  $\text{B-PRED}_{\mathcal{F}}$  can be solved in polynomial time: given  $F_\phi$ , an initial configuration  $(b, v)$  and a time  $t$ , it is sufficient to compute  $v' = v + t - 1 \bmod 2^n$  and verify the truth  $b'$  of  $\phi$  on valuation  $v'$  and we have  $(b', v' + 1 \bmod 2^n) = F^t(b, v)$ . To see that  $\text{PRED-CHG}_{\mathcal{F}}$  is NP-hard, it suffices to note that, on input  $(0, 0 \cdots 0)$ ,  $F_\phi$  will test successively each possible valuation for  $\phi$  and the state of node 1 will change to 1 at some time if and only if formula  $\phi$  is satisfiable.

For the second part of the proposition, the key is the construction for any  $n$  of an automata network  $H_n$  on  $Q^n$  that completely trivializes problem  $\text{PRED-CHG}$  in the following sense: for any configuration  $c \in Q^n$  and any  $k \leq 2^n$  and any node  $v$ , there is some  $t$  such that  $c_v \neq H_n^{kt}(c)_v$ . Taking any automata network  $F$  with  $n$  nodes, the product automata network  $F \times H_n$  (working on the product of alphabets in such a way that each component evolves independently) has the same property, namely that all instances of  $\text{PRED-CHG}$  with  $k \leq 2^n$  have a positive answer. From this, taking any family with a PSPACE-hard  $\text{PRED-CHG}$  problem (they are known to exist, see Corollary 1 for details), and replacing each automata network  $F$  with  $n$  nodes by the product  $F \times H_n$  (the circuit representation of the product is easily deduced from the representations of each component), we get a family  $(\mathcal{G}, \mathcal{G}^*)$  such that  $\text{B-PRED}_{\mathcal{G}}$  is **PSPACE**-complete while  $\text{PRED-CHG}_{\mathcal{G}}$  is easy: on one hand, taking products does not simplify  $\text{B-PRED}$  problem (because deciding whether node  $v$  is in state  $q$  on the  $F$  component reduces to deciding whether node  $v$  is in state  $(q, q')$  for some state  $q'$  of the  $H_n$  component); on the other hand,  $\text{PRED-CHG}$  becomes trivial (always true) on inputs where the observation interval  $k$  is less than  $2^n$ , and if  $k \geq 2^n$  then the size of the whole orbit graph of the input network is polynomial in  $k$  (since  $k$  is given in unary), so the entire orbit of the input configuration can be computed explicitly in polynomial time and the  $\text{PRED-CHG}$  can be answered in polynomial time.

Let us complete the proof by giving an explicit construction of the automata networks  $H_n$  over  $Q^n$  with the desired property.  $Q = \{0, 1\} \times \{0, 1\} \times \{0, 1\}$  and  $H_n$  interprets any configuration as a triplet of Boolean configurations  $(c, i, k)$  with the following meaning:  $k$  is a global counter that will take all possible values between 0 and  $2^n - 1$  and

loop,  $i$  is a local counter that will run from 0 to  $2k$  and  $c$  is the component where state changes will be realized at precise time steps to ensure the desired property of  $H_n$ . The goal is to produce in any orbit and for any  $k$  and at any node the sequence of states  $O^k 1^k$  on the  $c$ -component: such a behavior is sufficient to ensure the desired property on  $H_n$ . This is obtained by defining  $H_n(c, i, k) = (c', i', k')$  as follows:

- for any node  $v$ ,  $c'_v = 0$  if  $i < k$  or  $i \geq 2k$ , and  $c'_v = 1$  else,
- $i' = 0$  if  $i \geq 2k$  and  $i' + 1$  else,
- $k' = k + 1 \bmod 2^n$  if  $i \geq 2k$  and  $k' = k$  else.

It is clear that such an  $H_n$  admits a polynomial circuit representation **DLOGSPACE** computable from  $n$ . □

Finally, besides prediction problems, a classical type of problems studied in the literature are reachability problems [5, 4, 17]. Studying each variant of this type of problems goes beyond the scope of the present paper, but let us show that the most natural one is actually equivalent to **B-PRED** for general automata networks.

**Problem (Reachability (REACH)).**

**Parameters:** *alphabet  $Q$ , a standard representation  $\mathcal{F}^*$  of an automata network family  $\mathcal{F}$*

**Input:**

1. a word  $w_F \in \mathcal{F}^*$  representing an automata network  $F : Q^n \rightarrow Q^n$  on alphabet  $Q$ , with  $F \in \mathcal{F}$ .
2. an initial configuration  $x \in Q^V$ .
3. a target configuration  $y \in Q^V$ .

**Question:** *is there some  $t$  such that  $F^t(x) = y$ ?*

**Proposition 3.** *If we consider the family of all automata networks over some alphabet  $Q$  with circuit representations, then **B-PRED** and **REACH** are equivalent under **DLOGSPACE** reductions.*

*Proof.* Consider first an instance  $(F, v, x, q, t)$  of **B-PRED** and denote by  $n$  the number of nodes of  $F$  and  $m$  the maximum between  $n$  and the number of bits of the binary representation of  $t$ . It can be transformed into an instance  $(\overline{F}, x', y)$  of **REACH** in **DLOGSPACE** as follows.  $\overline{F}$  is a map  $A^m \rightarrow A^m$  where  $A = Q \times Q \times \{0, 1\} \cup \{\alpha\}$ . To simplify notation, we will write any configuration of  $A^m$  without occurrence of  $\alpha$  as  $(x, y, t)$  and see  $t$  as a number written in binary. Then  $\overline{F}$  is the following map:

$$\overline{F}(x, y, t) = \begin{cases} (x, F(y), t - 1) & \text{if } t > 0, \\ \alpha^m & \text{if } t = 0 \text{ and } x_v = q, \\ (x, y, 0) & \text{else,} \end{cases}$$

and  $\overline{F}$  is the identity on any other configurations, where  $F(y)$  denote the application of  $F$  on the first  $n$  nodes and the identity on the other ones. It is then straightforward to check that  $F^t(x)_v \neq x_v$  if and only if  $\overline{F}$  reaches configuration  $y = \alpha^m$  starting from configuration  $x' = (\overline{x}, \overline{x}, t)$  where  $\overline{x}$  is equal to configuration  $x$  on the  $n$  first nodes and fixed to an arbitrary constant on the remaining ones.

Conversely, any instance  $(F, x, y)$  of **REACH** can be transformed into an instance  $(\overline{F}, v, x, q, t)$  of **B-PRED** in **DLOGSPACE** as follows.  $\overline{F}$  is a map  $A^n \rightarrow A^n$  where  $n$  is the number of nodes of  $F$  and  $A = Q \times Q \times Q$ . Let us write any configuration of  $A^{n+1}$  as  $(x, y, t, a)$  where  $a \in A$  is the state of the  $(n + 1)$ -th node,  $(x, y, t)$  represent the content of the  $n$  first nodes on each component, and  $t$  is seen as a number between 0 and  $|Q|^n - 1$  written in base  $Q$ . Fix arbitrarily  $a_0 \neq a_1 \in A$ . Then  $\overline{F}$  is the following map:

$$\overline{F}(x, y, t, a) = \begin{cases} (F(x), y, t - 1, a) & \text{if } t > 0 \text{ and } x \neq y, \\ (F(x), y, t - 1, a_1) & \text{if } t > 0 \text{ and } x = y, \\ (y, y, 0, a) & \text{if } t = 0 \text{ and } x \neq y, \\ (y, y, 0, a_1) & \text{if } t = 0 \text{ and } x = y. \end{cases}$$

One can check that  $F$  reaches  $y$  starting from  $x$  if and only if  $\overline{F}^{|Q|^n}(x, y, |Q|^n - 1, a_0)$  is of the form  $(*, *, *, a_1)$ , hence a reduction of  $\text{REACH}_F$  to  $\text{B-PRED}_{\overline{F}}$ . Indeed, if  $F$  ever reaches  $y$  from  $x$ , it must be at step  $t$  with  $0 \leq t \leq |Q|^n - 1$  and the behavior of  $\overline{F}$  consists exactly in testing if at any steps equality  $x = y$  holds and then memorize this in the  $(n + 1)$ -th node. Moreover,  $\overline{F}$  always converges in at most  $|Q|^n$  steps to a fixed point of the form  $(y, y, 0, a)$ .  $\square$

The above equivalence works in general, but may fail for particular families as shown below.

**Theorem 11.** *There exists a family with circuit representation  $(\mathcal{F}, \mathcal{F}^*)$  such that  $\text{B-PRED}_{\mathcal{F}}$  and  $\text{PRED-CHG}_{\mathcal{F}}$  are NP-hard while  $\text{REACH}_{\mathcal{F}}$  is solvable in polynomial time. Conversely, there exists a family with circuit representation  $(\mathcal{G}, \mathcal{G}^*)$  such that  $\text{REACH}_{\mathcal{G}}$  is PSPACE-complete while  $\text{PRED-CHG}_{\mathcal{G}}$  is solvable in polynomial time.*

*Proof.* For each  $n$  and each SAT formula  $\phi$  with  $n$  variables let us define  $F_\phi : \{0, 1\}^{n+1} \rightarrow \{0, 1\}^{n+1}$  which interprets any configuration as a pair  $(b, v) \in \{0, 1\} \times \{0, 1\}^n$  where  $b$  is the state of node 1 and  $v$  is both a number represented in base 2 and a valuation for  $\phi$  and does the following:

$$F_\phi(b, v) = \begin{cases} (0, v + 1 \bmod 2^n) & \text{if } b = 1 \text{ or } (b = 0 \text{ and } \neg\phi(v)) \\ (1, v) & \text{else.} \end{cases}$$

Note that circuits computing  $F_\phi$  can be constructed in **DLOGSPACE** from  $\phi$ . We thus have a well-defined family with circuit representation. A configuration  $(b, v)$  is reachable (from any initial configuration) if and only if either  $b = 0$ , or if  $b = 1$  and  $\neg\phi(v)$ .  $\text{REACH}_{\mathcal{F}}$  is therefore solvable in polynomial time in  $n$ .

However, node 1 will change its state in the orbit of configuration  $(0, v)$  (for some arbitrary  $v \in \{0, 1\}^n$ ) if and only if  $\phi$  is satisfiable. Besides, it holds from the definition above that  $F_\phi^{2^n}(0, v) = (0, v)$  if and only if there is no configuration of the form  $(1, v')$  in the orbit of  $(0, v)$ , *i.e.* if and only if  $\phi$  is not satisfiable. We deduce that  $\text{B-PRED}_{\mathcal{F}}$  is NP-hard.

The construction of family  $(\mathcal{G}, \mathcal{G}^*)$  making  $\text{REACH}_{\mathcal{G}}$  hard and  $\text{PRED-CHG}_{\mathcal{G}}$  easy is inspired from the construction of Theorem 10. Taking any  $F_n : Q_F^n \rightarrow Q_F^n$ , we will use again the automata network  $H_n : Q_H^n \rightarrow Q_H^n$  from the proof of Theorem 10, and we construct  $G_n : (Q_F \times Q_H)^n \rightarrow (Q_F \times Q_H)^n$  defined by:

$$G_n(c_F, c_H) = \begin{cases} (F_n(c_F), H_n(c_H)) & \text{if } c_H \text{ is of the form } (0, 0, 0), \\ (c_F, H_n(c_H)) & \text{else.} \end{cases}$$

So  $G_n$  is just  $H_n$  on the  $Q_H$  component. Moreover, it can be checked that  $H_n$  starting from  $c_0 = (0, 0, 0)$  goes back to  $c_0$  after some time  $T_0$ . Thus when  $G_n$  is started from some configuration  $(x, c_0)$  it reaches  $(F_n^t(x), c_0)$  after  $tT_0$  time steps (for any  $t \geq 1$ ) and no other configuration in this orbit is equal to  $c_0$  on the second component. We deduce that  $F_n$  reaches configuration  $y$  starting from configuration  $x$  if and only if  $G_n$  reaches  $(y, c_0)$  from configuration  $(x, c_0)$ . By choosing the family of networks  $F_n$  with PSPACE-hard reachability, we obtain the family  $(\mathcal{G}, \mathcal{G}^*)$  with the desired properties.  $\square$

As a last 'orthogonality' result, let us show that a bound on a single dynamical parameter (periods or transients) is generally not sufficient to discard maximal computational complexity, while a bound on both periods and transients is.

**Theorem 12.** *For any family  $(\mathcal{F}, \mathcal{F}^*)$  where all periods and all transients are polynomially bounded by the number of nodes, the problems  $\text{REACH}_{\mathcal{F}}$ ,  $\text{PRED-CHG}_{\mathcal{F}}$  and  $\text{B-PRED}_{\mathcal{F}}$  are solvable in polynomial time. However there exists a family with circuit representation  $(\mathcal{G}, \mathcal{G}^*)$  made only of reversible automata networks (*i.e.* having only periodic orbits and no transients) such that  $\text{B-PRED}_{\mathcal{G}}$  is PSPACE-complete. There exists also a family with circuit representation  $(\mathcal{H}, \mathcal{H}^*)$  made of automata networks whose only periodic orbits are fixed points such that  $\text{B-PRED}_{\mathcal{H}}$  is PSPACE-complete.*

*Proof.* First, if all periods and transients are polynomially bounded, then there is a PTIME algorithm that given an initial configuration computes the (polynomial) list of configurations that are in its limit period and the first time at which they are reached. From this information it is straightforward to solve problems  $\text{REACH}_{\mathcal{F}}$ ,  $\text{PRED-CHG}_{\mathcal{F}}$  and  $\text{B-PRED}_{\mathcal{F}}$  in PTIME.

For the second assertion of the theorem, let us recall that any deterministic Turing machine working in space  $S$  and time  $T$  no more than exponential can be simulated by a deterministic reversible Turing machine in time

polynomial in  $T$  and space polynomial in  $S$  [6, 36]. By deterministic reversible Turing machine, we mean a machine whose transition graph has in-degree and out-degree at most 1, *i.e.* any Turing configuration (tape, head state and position) has 0 or 1 successor configuration (for instance 0 in the case of an halting state) and 0 or 1 predecessor. Let us therefore consider a fixed deterministic reversible machine  $M$  working in space  $N(n) \in poly(n)$ , that solves the truth problem for quantified boolean formulas (QBF) in time  $k^{N(n)}$  where  $k$  is a constant and  $n$  is the size of the QBF instance. By using an additional counter mechanism we can delay arbitrarily the time at which the machine enters an halting state after the QBF computation has been done, precisely: we can suppose without loss of generality that the machine writes somewhere the acceptance information (truth of the QBF formula) of any well formed input in time *at most*  $(k/2)^{N(n)}$  and leaves it untouched during *at least*  $(k/2)^{N(n)}$  additional steps before entering an halting state. This means that from any well-formed input configuration, the machine runs for at least  $(k/2)^{N(n)}$  steps without halting (each configuration has a successor) and at time exactly  $(k/2)^{N(n)}$ , the configuration always contains the information of the acceptance of the QBF input. For some large enough constant alphabet  $Q$  and for each  $n$ , we can construct an automata network  $G_n : Q^{N(n)+1} \rightarrow Q^{N(n)+1}$  where the  $N(n)$  first nodes are used to simulate  $M$  on QBF instances of size  $n$ , and the last node holds two Boolean informations: the simulation direction (forward or backward) and an acceptance bit.  $G_n$  behaves as follows on any configuration  $x \in Q^{N(n)+1}$ :

- if  $x$  is not well encoded and does not represent a valid Turing configuration (tape, head position within space bounds and head state), then let it unchanged ( $x$  is a fixed point);
- if the  $N(n)$  first nodes (correctly) encode a configuration with no successor (resp. predecessor) and node  $N(n) + 1$  indicates the forward (resp. backward) direction, then change the direction and let the encoded configuration unchanged;
- finally if the (correctly) encoded configuration has a successor (resp. predecessor) and node  $N(n) + 1$  indicates the forward (resp. backward) direction, then do one step of simulation, let the direction unchanged and update the acceptance bit according to the new configuration obtained.

By reversibility of  $M$ ,  $G_n$  is itself reversible. Precisely,  $G_n$  has only periodic orbits, which are of three kinds: 'garbage' fixed points that do not correspond to any valid configuration of  $M$  because of bad encoding, periodic orbits corresponding to periodic orbits of  $M$  (without halt), and periodic orbits that correspond to a loop of back and forth simulation of a single orbit of  $M$  that starts from a configuration without predecessor and ends in a configuration without successor. Moreover, on any well formed input configuration  $x$  representing a QBF  $\phi$  of size  $n$ , it holds that the acceptance bit of node  $N(n) + 1$  in  $F^{(k/2)^{N(n)}}(x)$  tells whether  $\phi$  is true or not. We deduce that  $\mathbf{B-PRED}_{\mathcal{G}}$  is PSPACE-complete where  $\mathcal{G}$  is the family of networks  $G_n$  with circuit representation (a circuit representation for  $G_n$  is easy to compute from  $n$  since  $M$  is fixed).

For the last claim of the theorem, take any family with a PSPACE-hard  $\mathbf{B-PRED}$  problem and transform it into a new family where each automata network is simulated step by step by a new one that implements an additional  $k$ -ary counter layer in states that is decreased at each simulation steps, and that stops the simulation and forces a fixed point when value zero is reached. Such networks have only fixed point by construction, and for a suitable choice of constant  $k$ , the PSPACE-hardness of  $\mathbf{B-PRED}$  is preserved because on well initialized configurations, the counter mechanism still allows an exponential number of simulation steps.  $\square$

## 4.4 Universal automata network families

Building upon our definition of simulation, we can now define a precise notion of universality. In simple words, an universal family is one that is able to simulate every other automata network under any circuit encoding. Our definition of simulation ensures that the amount of resources needed in order to simulate is controlled so that we can deduce precise complexity results.

Consider some alphabet  $Q$  and some polynomial map  $P : \mathbb{N} \rightarrow \mathbb{N}$ . We denote by  $\mathcal{U}_{Q,P}$  the class of all possible functions  $F : Q^n \rightarrow Q^n$  for any  $n \in \mathbb{N}$  that admits a circuit representation of size at most  $P(n)$ . We also denote  $\mathcal{U}_{Q,P}^*$  the language of all possible circuit representations of size bounded by  $P$  of all functions from  $\mathcal{U}_{Q,P}$ . First, note that any family with standard representation  $(\mathcal{F}, \mathcal{F}^*)$  is actually simulated by  $(\mathcal{U}_{Q,P}, \mathcal{U}_{Q,P}^*)$  for some  $P$  because the definition of standard representation implies that there is a  $\mathbf{DLOGSPACE}$  algorithm to produce a circuit representation of a given automata network of family  $\mathcal{F}$  from its representation. The notion of universality is about simulations in the other direction.

Finally for any  $\Delta \geq 1$ , denote by  $\mathcal{B}_{Q,\Delta}$  the set of automata networks on alphabet  $Q$  with a communication graph of degree bounded by  $\Delta$  and by  $\mathcal{B}_{Q,\Delta}^*$  their associated bounded degree representations made of a pair (graph, local maps) as discussed above. They form a smaller set of automata networks that may be simulated more tightly, which is the idea of the notion of strong universality.

**Definition 13.** *A family of automata networks  $(\mathcal{F}, \mathcal{F}^*)$  is :*

- universal if for any alphabet  $Q$  and any polynomial map  $P$  it can simulate  $(\mathcal{U}_{Q,P}, \mathcal{U}_{Q,P}^*)$  in time  $T$  and space  $S$  where  $T$  and  $S$  are polynomial functions;
- strongly universal if for any alphabet  $Q$  and any degree  $\Delta \geq 1$  it can simulate  $(\mathcal{B}_{Q,\Delta}, \mathcal{B}_{Q,\Delta}^*)$  in time  $T$  and space  $S$  where  $T$  is a constant and  $S$  is a linear map.

**Remark 6.** *The link between the size of automata networks and the size of their representation is the key in the above definitions: a universal family must simulate any individual automata network  $F$  (just take  $P$  large enough so that  $F \in \mathcal{U}_{Q,P}$ ), however it is not required to simulate in polynomial space and time the family of all possible networks without restriction. Actually no family admitting polynomial circuit representation could simulate the family of all networks in polynomial time and space by the Shannon effect (most  $n$ -ary Boolean function have super-polynomial circuit complexity). In particular the family  $\mathcal{B}_{Q,\Delta}$  can't.*

*At this point it is clear, by transitivity of simulations, that if some  $\mathcal{B}_{Q,\Delta}$  happens to be universal then, any strongly universal family is also universal. It turns out that  $\mathcal{B}_{\{0,1\},3}$  is universal. We will however delay the proof of this result until the second paper of this series, where we show a more precise result. Moreover, we show in fact a very useful result that gives sufficient conditions for universality in concrete families.*

*Finally, observe that universality allows a polynomial spatio-temporal rescaling, while strong universality allows only constant one. The fact that  $S$  and  $T$  are polynomial maps implies that they are computable in **DLOGSPACE** which is coherent with the reductions presented in Lemma 8 and Lemma 9.*

Now, we introduce an important corollary of universality regarding complexity. Roughly speaking, a universal family exhibits all the complexity in terms of dynamical behaviour and computational complexity of prediction problems. Concerning computational complexity, we state the result for universality, but there is actually no difference between strong or standard universality since the former implies the later as we will see in the second paper of this series [46, Corollary 3].

**Corollary 1.** *Let  $(\mathcal{F}, \mathcal{F}^*)$  be a universal automata network family, then it is computationally complex in the following sense:*

1.  $U\text{-PRED}_{\mathcal{F}}$  is **P-hard**.
2.  $B\text{-PRED}_{\mathcal{F}}$  is **PSPACE-hard**.
3.  $PRED\text{-CHG}_{\mathcal{F}}$  is **PSPACE-hard**.
4.  $REACH_{\mathcal{F}}$  is **PSPACE-hard**.

*Proof.* We first show that the family  $\mathcal{B}_{Q,\Delta}$  is computationally complex for all problems except REACH and large enough  $Q$  and  $\Delta$ , which shows the hardness results of the three first problems by definition of universality and Lemmas 8 and 9. First, any Turing machine working in bounded space can be directly embedded into a cellular automaton on a periodic configuration which is a particular case of automata network on a bounded degree communication graph (for the PRED-CHG variant we can always add a witness node that changes only when the Turing machine accepts for instance). This direct embedding is such that one step of the automata network correspond to one step of the Turing machine and one node of the network corresponds to one cell of the Turing tape. However, the alphabet of the automata network depends on the tape alphabet and the state set of the Turing machine. To obtain the desired result we need to fix the target alphabet, while allowing more time and/or more space. Such simulations of any Turing machine by fixed alphabet cellular automata with linear space/time distortion are known since a long time [35], but a modern formulation would be as follows: if there exists an intrinsically universal cellular automaton [11] with states set  $Q$  and neighborhood size  $\Delta$  (whatever the dimension), then  $\mathcal{B}_{Q,\Delta}$  is computationally complex. The 2D cellular automaton of Banks [3] is intrinsically universal [44] and has two states and 5 neighbors, which shows that  $\mathcal{B}_{Q,\Delta}$  is computationally complex when  $\Delta \geq 5$  and  $Q$  is not a singleton. The 1D intrinsically universal

cellular automaton of Ollinger-Richard [45] has 4 states and 3 neighbors so  $\mathcal{B}_{Q,\Delta}$  is computationally complex when  $\Delta \geq 3$  and  $|Q| \geq 4$ . Finally,  $\text{REACH}_{\mathcal{F}}$  is also **PSPACE**-hard because Proposition 3 shows that  $\text{REACH}_{\mathcal{F}}$  is as hard as  $\text{B-PRED}_{\mathcal{U}_{Q,P}}$  for any large enough  $P$ , and this latter problem is **PSPACE**-hard because  $\text{B-PRED}_{\mathcal{B}_{Q,\delta}}$  is and Lemma 8 applies since  $\mathcal{U}_{Q,P}$  clearly simulates  $\mathcal{B}_{Q,\Delta}$ .  $\square$

We now turn to the dynamical consequences of universality. By definition simulations are particular embeddings of orbit graphs into larger ones, but the parameters of the simulation can generate some distortion and the set of orbit graphs that can be embedded have succinct descriptions by circuits. Before stating the main theorem, let us give some definitions to clarify these aspects.

**Definition 14.** Fix a map  $\rho : \mathbb{N} \rightarrow \mathbb{N}$ , we say that the orbit graph  $G_F$  of  $F$  with  $n$  nodes is  $\rho$ -succinct if  $F$  can be represented by circuits of size at most  $\rho(n)$ . We say that the orbit graph  $G_H$  of  $H$  with  $m$  nodes embeds  $G_F$  with distortion  $\delta : \mathbb{N} \rightarrow \mathbb{N}$  if  $m \leq \delta(n)$  and there is  $T \leq \delta(n)$  such that  $G_F$  is a subgraph of  $G_{HT}$ .

**Remark 7.** The embedding of orbit graphs with distortion obviously modify the relation between the number of nodes of the automata networks and the length of paths or cycles in the orbit graph. In particular, with polynomial distortion  $\delta$ , if  $F$  has  $n$  nodes and a cyclic orbit of length  $2^n$  (hence exponential in the number of nodes) then in  $H$  it gives a cyclic orbit of size  $O(\delta(n)2^n)$  for up to  $\delta(n)$  nodes, which does not guarantee an exponential length in the number of nodes in general, but just a super-polynomial one ( $n \mapsto 2^{n^\alpha}$  for some  $0 < \alpha < 1$ ).

To fix ideas, we give examples of orbit graphs of bounded degree automata networks with large components corresponding to periodic orbits or transient.

**Proposition 4.** There is an alphabet  $Q$  such that for any  $n \geq 1$  there is an automata network  $F_n \in \mathcal{B}_{Q,2}$  whose orbit graph  $G_{F_n}$  has the following properties:

- it contains a cycle  $C$  of length at least  $2^n$ ;
- there is a complete binary tree  $T$  with  $2^n$  leaves connected to some  $v_1 \in C$ , i.e. for all  $v \in T$  there is a path from  $v$  to  $v_1$ ;
- there is a node  $v_2 \in C$  with a directed path of length  $2^n$  pointing towards  $v_2$ ;
- it possesses at least  $2^n$  fixed points.

*Proof.* First on a component of states  $\{0, 1, 2\} \subseteq Q$  the large cycle  $C$  is obtained by the following 'odometer' behavior of  $F_n$ : if  $x_n \in \{0, 1, 2\}$  then  $F_n(x)_n = x_n + 1 \pmod 3$ , and if both  $x_i, x_{i+1} \in \{0, 1, 2\}$  for  $1 \leq i < n$  then

$$F_n(x)_i = \begin{cases} 0 & \text{if } x_i = 2 \\ x_i + 1 & \text{else if } x_{i+1} = 2, \\ x_i & \text{else.} \end{cases}$$

$C$  is realized on  $\{0, 1, 2\}^n$  as follows. For  $x \in \{0, 1, 2\}^n$  denote by  $S_i$  the sequence  $(F^t(x)_i)_{t \geq 0}$  for any  $1 \leq i \leq n$ . Clearly  $S_n$  is periodic of period 012.  $S_{n-1}$  is ultimately periodic of period 200111 (of length 6) and by a straightforward induction we get that  $S_1$  is ultimately periodic of period  $20^{3 \cdot 2^{n-2} - 1} 1^{3 \cdot 2^{n-2}}$  which is of length  $3 \cdot 2^{n-1}$ .

For the tree  $T$ , just add states  $\{a, b\} \subseteq Q$  with the following behavior: if  $x_1 \in \{a, b\}$  then  $F_n(x)_1 = 0$  and if  $x_i \in \{a, b\}$  and  $x_{i-1} = 0$  then  $F_n(x)_i = 0$  for  $1 < i \leq n$ . In any other case, we set  $F(x)_i = x_i$  for  $x \in \{0, 1, 2, a, b\}^n$  and  $1 \leq i \leq n$ .

Using similar mechanisms as above on additional states  $c_0, c_1, c_2 \in Q$ ,  $F_n$  runs another odometer whose behavior is isomorphic to the behavior of  $F_n$  on  $\{0, 1, 2\}^n$  through  $i \mapsto c_i$ , but with the following exception: when  $x_1 = c_2$  we set  $F_n(x)_1 = 0$  and then state 0 propagates from node 1 to node  $n$  as in the construction of tree  $T$ . We thus get a transient behavior of length more than  $3 \cdot 2^{n-1}$  which yields to configuration  $0^n$ , which itself (belongs or) yields to cycle  $C$ .

Finally, the fixed points are obtained by adding two more states to the alphabet on which the automata network just acts like the identity map.  $\square$

We can now state that any universal family must be dynamically rich in a precise sense.

**Theorem 15.** *Let  $\mathcal{F}$  be an automata networks family.*

- *If  $\mathcal{F}$  is universal then, for any polynomial map  $\rho$ , there is a polynomial distortion  $\delta$  such that, any  $\rho$ -succinct orbit graph can be embedded into some  $F \in \mathcal{F}$  with distortion  $\delta$ . In particular  $\mathcal{F}$  contains networks with super-polynomial periods and transients, and a super-polynomial number of disjoint periodic orbits of period at most polynomial.*
- *If  $\mathcal{F}$  is strongly universal then it embeds the orbit graph of any bounded-degree automata network with linear distortion. In particular it contains networks with exponential periods and transients, and an exponential number of disjoint periodic orbits of period at most linear.*

*Proof.* This is a direct consequence of Lemma 6, Definition 7 and Proposition 4 above. □

Of course, we do not claim that computational complexity and dynamical richness as stated above are the only meaningful consequences of universality. To conclude this subsection about universality, let us show that it allows to prove finer results linking the global dynamics with the interaction graph.

In a directed graph, we say a node  $v$  belongs to a strongly connected component if there is a directed path from  $v$  to  $v$ .

**Corollary 2.** *Any universal family  $\mathcal{F}$  satisfies the following: there is a constant  $\alpha$  with  $0 < \alpha \leq 1$  such that for any  $m > 0$  there is a network  $F \in \mathcal{F}$  with  $n \geq m$  nodes such that some node  $v$  belonging to a strongly connected component of the interaction graph of  $F$  and a periodic configuration  $x$  such that the trace at  $v$  of the orbit of  $x$  is of period at least  $2^{n^\alpha}$ .*

*Proof.* Consider a Boolean network  $F$  with nodes  $V = \{1, \dots, m\}$  that do the following on configuration  $x \in \{0, 1\}^V$ : it interprets  $x_1, \dots, x_m$  as an number  $k$  written in base 2 where  $x_1$  is the most significant bit and produces  $F(x)$  which represents number  $k + 1 \pmod{2^m}$ .

$F$  is such that node 1 has a trace of exponential period and belongs to a strongly connected component of the interaction graph of  $F$  (because it depends on itself). Note that  $F$  has a circuit representation which is polynomial in  $m$ , and take  $F' \in \mathcal{F}$  of size polynomial in  $m$  that simulates  $F$  in polynomial time (by universality of family  $\mathcal{F}$ ). Taking the notations of Definition 5, we have that each node  $v \in D_i$  for each block  $D_i$  is such that the map  $q \in \{0, 1\} \mapsto p_{i,q}(v)$  is either constant or bijective (because  $F$  has a Boolean alphabet, see Remark 3). In the last case, the value of the node  $v \in D_i$  completely codes the value of the corresponding node  $i$  in  $F$ . Take any  $v \in B_1$  that has this coding property. Since node 1 depends on itself in  $F$ , there must be a path from  $v$  to some node  $v' \in D_1$  that is also coding in the interaction graph of  $F'$ . Then we can also find a path from  $v'$  to some coding node in  $D_1$ . Iterating this reasoning we must find a cycle, and in particular we have a coding node in  $D_1$  which belongs to some strongly connected component of the interaction graph of  $F'$ . Since this node is coding the values taken by node 1 of  $F$  and since the simulation is in polynomial time and space, we deduce the super-polynomial lower bound on the period of its trace for a well-chosen periodic configuration. □

## 4.5 Link with cellular automata and intrinsic universality

A cellular automaton is essentially an infinite automata network which is uniform both in the communication graph and the local rule of nodes. Let  $d \geq 1$  be an integer and  $N \subseteq \mathbb{Z}^d$  be a finite set. A cellular automaton of dimension  $d$  and neighborhood  $N$  and state set  $Q$  is defined by a local rule  $\delta : Q^N \rightarrow Q$  which induces a global map  $F_\delta : Q^{\mathbb{Z}^d} \rightarrow Q^{\mathbb{Z}^d}$  defined as follow:

$$F_\delta(c)_z = \delta(z' \in N \mapsto c_{z+z'}).$$

One can naturally associate to such a cellular automaton a family of automata networks defined over regular graphs that are  $d$ -dimensional tori with uniform adjacency relation defined by  $N$ , and such that each node has the same local rule  $\delta$ . Formally, for any  $n \in \mathbb{N}$ , let  $G_{d,N,n}$  be the graph of vertex set  $V_{d,n} = \mathbb{Z}_n^d$  where  $\mathbb{Z}_n$  denotes the integers modulo  $n$ , and such that  $(i, j) \in V_{d,n}^2$  is an edge if and only if  $j - i \in N$  (where the computation is done

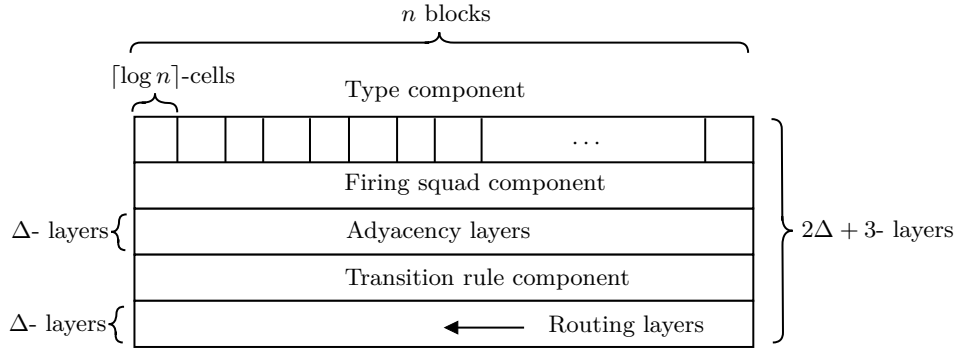


Figure 9: Representation of the coding of an arbitrary graph by a one dimensional cellular automata as it is described in Theorem 17

modulo  $n$ ). For large enough  $n$ ,  $G_{d,N,n}$  is a regular graph of degree  $|N|$ . Then, on each  $G_{d,N,n}$ , we consider the automata network where the local rule of each node  $i$  is  $\delta$  where we identify the neighborhood of  $i$  to  $N$  by  $j \mapsto j - i$  (which is one-to-one for large enough  $n$ , the choice for a constant number of small values of  $n$  does not matter). We denote this family  $\mathcal{F}_{d,N,Q,\delta}$  and consider it together with its bounded-degree representation.

A well-established notion of universality in cellular automata, *intrinsic universality*, is actually very close to our formalism and relies on the notion of *intrinsic simulations*. The goal of this subsection is to clarify the links between intrinsic universality of a cellular automaton, and universality of the associated automata networks family.

To be precise we consider the notion of intrinsic universality [11, Definition 5.1] associated to injective simulation [11, Definition 2.1]. The definition of injective simulation between  $d$ -dimensional cellular automata is essentially equivalent to Definition 5 with the additional constraint that the block embedding uses the same 'rectangular' shape for all blocks. We say that a block embedding between automata networks over graphs  $G_{d,N_1,n_1}$  and  $G_{d,N_2,n_2}$  is a *uniform rectangular block embedding* of shape  $\vec{b} = (b_1, \dots, b_d)$  if it is such that each block  $D_i$  is of the form  $v_i + [0, \dots, b_1] \times \dots \times [0, \dots, b_d]$  for some  $v_i$ . Injective intrinsic universality of cellular automata can then be defined on the associated automata network families as follows.

**Definition 16.** A cellular automaton of dimension  $d$ , neighborhood  $N$ , state set  $Q$  and local rule  $\delta$  is intrinsically universal if for any neighborhood  $N'$ , state set  $Q'$  and local rule  $\delta'$ , the family  $\mathcal{F}_{d,N,Q,\delta}$  simulates  $\mathcal{F}_{d,N',Q',\delta'}$  in constant time and with a uniform rectangular block embedding of fixed shape  $\vec{b}$ .

As a first result, let us show that intrinsic universality implies a very general capacity of simulating automata networks, close to strong universality but slightly weaker.

**Theorem 17.** Consider any  $d$ -dimensional intrinsically universal CA and denote by  $(\mathcal{F}, \mathcal{F}^*)$  its associated automata network family with bounded degree representation. For any  $Q$  and  $\Delta$ ,  $\mathcal{F}$  can simulate  $\mathcal{B}_{Q,\Delta}$  in time  $O(n \log(n))$  and space  $O(n \log(n))$ .

*Proof.* We do the proof for dimension 1, it is straightforward to lift the construction to higher dimension by periodization in all but one dimensions. It is sufficient to prove that some family  $\mathcal{F}_{1,\{-1,0,1\},Q',\delta}$  associated to a cellular automaton can simulate  $\mathcal{B}_{Q,\Delta}$  in time  $O(n \log(n))$  and space  $O(n \log(n))$  for each fixed choice of  $Q$  and  $\Delta$ . When  $Q$  and  $\Delta$  are fixed, there are only finitely many possible local transition rules so, by choosing  $Q'$  large enough, any such rule can be encoded locally as well as the set of possible values  $Q^\Delta$  of the neighbors of a given node. The only difficulty of the simulation lies in the routing of states of nodes to their corresponding neighbors according to an arbitrary graph of degree  $\Delta$ . The main trick is that the communication of the state of each node to each of its neighbors is done by a routing mechanism of packets turning on a cycle graph: each holds a number coding the travel distance it has to accomplish before delivering its information (a state), and, while turning on the cycle, each packet decrements its number until it is 0 and then triggers the information delivery. Let us describe a cellular automaton of dimension 1 of local rule  $\delta$  that can achieve this routing task and the complete simulation. Let us fix any network from  $\mathcal{B}_{Q,\Delta}$  with  $n$  nodes and communication graph  $G$ . It is simulated by the cellular automaton on the graph  $G_{1,\{-1,0,1\},n \log(n)}$  as follows:

- each node of  $G$  is simulated by a block of  $\lceil \log(n) \rceil$  adjacent cells of the 1D cellular automaton, the  $i$ th blocks corresponds to the  $i$ th node;



- the alphabet  $Q'$  is structured in  $2\Delta + 3$  components:
  - a *type* component that serves as a marker on some cells to give them a particular behavior, or mark the limits of each block, called block skeleton; this component is invariant;
  - a *firing squad* component [51] that serves as a global clock for the simulation that “ticks” every  $O(n \log(n))$  steps by having a special “fire” flag appear at every cells exactly at these time steps (it is well-known that such a periodic behavior can be realized by a firing squad with a linear relation between the number of cells and the time period [51]);
  - a *transition rule* component that can hold the complete information about the transition rule of a simulated node, its state and the states of its neighbors; more precisely, this layer is empty, except for the rightmost position of each block of the skeleton where it is initialized with empty information about neighbors, just the state and the local rule of the simulated node corresponding to the block;
  - $\Delta$  *graph adjacency* components, that remain constant and that describe the adjacency relation of graph  $G$ : for each block  $i$ , each such component gives one neighbor of  $i$  by coding, as a number written in binary from (less significant bit at the leftmost position), the distance in blocks starting from block  $i$  to reach block  $j$ ;
  - $\Delta$  *routing* components that are each organized as blocks of  $\lceil \log(n) \rceil$  states, called *packet*, that each hold a number (the address), that is initially aligned with the block skeleton, and initialized by the content of the graph adjacency components; moreover, the rightmost cell of the packet holds a state from  $Q$  plus an index between 1 and  $\Delta$  (the data); the role of each packet is to send the state of a node to one of its neighbors;
- all packets shift “to the left” (from position  $p$  to  $p - 1$  in the graph  $G_{1, \{-1, 0, 1\}, n \log(n)}$ ) synchronously cell by cell and each packet perform the following task as it travels: when the leftmost cell of a packet encounters the right boundary of block of the skeleton, it starts to decrement the number held in the packet by propagating a  $-1$  carry that travels from left to right; if the carry reaches the rightmost position of the packet (meaning the number was 0 and cannot be decremented), then it means that the packet has reached the block of the skeleton corresponding to its initial address: in this case the rightmost position of the packet transmits to the transition rule component of the rightmost cell of the block of the skeleton all its data exactly when it receives the carry and is aligned with the right boundary of the block; after this, the packet still travels by shifts but is deactivated so that all packets are deactivated and have correctly transmitted their data after  $n \log(n)$  steps.
- the synchronous global clock achieved by the firing squad layer triggers two operations on other layers when it ticks: it forces the transition rule component to actually compute one transition and clean the local information about states of neighbors ; and it reset the routing component according to the graph adjacency component (for the address in packets) and the transition rule component (for the data of the packets). This cleaning process is done in one step since each node sees locally the special state of the firing squad and erases the layers to be cleaned locally in one step.

The block embedding of the simulation is very regular: each node  $i$  of  $G$  is represented by the  $i$ th block in the skeleton, with the firing squad layer initialized in the state obtained just after the “fire” step, the transition rule component holding only local states and transition rule of each node and no information about the neighbors, and the routing components initialized according to the graph adjacency components. By the description of the behavior above, in  $n \log(n)$  steps, all packets have visited the entire block skeleton so they have all copied their information to the corresponding slots of the transition table component and are deactivated. After  $O(n \log(n))$  steps the firing squads component fires, the correct transitions are computed everywhere and we are back to a well-formed block encoding representing the new configuration of nodes of graph  $G$ .  $\square$

**Remark 8.** *As shown in the second paper of this series[46], the simulation result of Theorem 17 is enough to give universality: any automata network family (with bounded degree representation) associated to some  $d$ -dimensional intrinsically universal CA is actually universal. Precisely, such a family simulates the family  $\mathcal{G}_m$  (a subfamily of  $\mathcal{B}_{\{0,1\},4}$  defined in [46]) in time  $O(n \log(n))$  and space  $O(n \log(n))$  by Theorem 17. Such a simulation of  $\mathcal{G}_m$  is sufficient for universality [46, Theorem 17].*

Let us now prove that a family of automata networks coming from a  $d$ -dimensional cellular automaton cannot be strongly universal, whatever the cellular automaton considered. The reason is that the rigidity of the network of the cellular automaton limits propagation of information and prevents a simulation with constant spatio-temporal rescaling factors of networks on arbitrary graphs. To show this, we will use the notion of growth of balls in graph

families. Given a family of finite graphs  $(G_i)_{i \in I}$ , we say that it has a *polynomial ball growth* if there is some exponent  $k \in \mathbb{N}$  such that for any fixed  $m$  there is a constant  $C_m$  such that for any  $i \in I$  and set  $X$  of  $m$  vertices of  $G_i$ :

$$\forall n, |B(X, n)| \leq C_m n^k$$

where  $B(X, n)$  denotes the set of nodes at distance  $n$  from  $X$  in  $G_i$ . The family of  $d$ -dimensional grids has polynomial ball growth, while the family of binary trees hasn't.

Let  $\mathcal{F}$  be a network family. We say that  $\mathcal{F}$  has polynomial ball growth if the family of its underlying communication graphs has polynomial ball growth.

**Theorem 18.** *No family of polynomial ball growth can be strongly universal.*

*Proof.* Consider the family  $\mathcal{F}_0$  of disjunctive networks on complete binary trees with self-loops, and let  $\mathcal{F}$  be any family with polynomial ball growth (details about representations don't matter for the argument). Suppose for the sake of contradiction that  $\mathcal{F}$  simulates  $\mathcal{F}_0$  with constant spatio-temporal rescaling:  $t$  steps of an automata network  $F_0$  of size  $n$  from  $\mathcal{F}_0$  are simulated in time at most  $\alpha t$  by an automata network  $F$  of size at most  $\alpha n$  from  $\mathcal{F}$ . The configuration everywhere 0 is a fixed point of  $F_0$  so its block encoding must be a fixed point of  $F$ . Let's call it  $c_0$ . In any case, there are some nodes of  $F_0$  which are simulated by a block of nodes of  $F$  of size at most  $\alpha$ . Choose any such node  $v$  and consider the configuration of  $F_0$  which is everywhere 0 except on this node  $v$  where it is 1. Since the graph of  $F_0$  is a complete binary tree, in  $\log(n)$  steps the considered configuration becomes the configuration everywhere 1 under the action of  $F_0$ . On the other hand, these  $\log(n)$  steps must be simulated by  $F$  in at most  $\alpha \log(n)$  steps, starting from a configuration  $c_1$  which differs from  $c_0$  only on the block  $D_v$  of size at most  $\alpha$ . In the orbit of  $c_1$ , after  $t$  steps, only the nodes of  $F$  that are at distance at most  $t$  from  $D_v$  can be in a different state than in  $c_0$ . By the polynomial ball growth of exponent  $k$  with  $m = \alpha$  there are at most  $C_m \log^k(n)$  nodes that differ between  $c_0$  and  $F^{\log(n)}(c_1)$ . For  $n$  large enough, this is not sufficient to have  $n$  blocks to change the state they represent as they should to correctly simulate the  $n$  nodes of  $F_0$ .  $\square$

**Corollary 3.** *No automata network family coming from a  $d$ -dimensional cellular automaton can be strongly universal.*

*Proof.* It follows directly from Theorem 18 because for any  $d$  and  $N$ , the family of graphs  $(G_{d,N,n})_{n \in \mathbb{N}}$  is of polynomial ball growth.  $\square$

## 5 Perspectives

The main contribution of this paper is a general formalism of intrinsic universality for families of automata networks, with all the dynamical and computational consequences such a notion implies (which can be seen as necessary conditions for universality). As announced earlier, this paper is the first of a series of three and the main continuations of the present work are:

- establishing sufficient conditions for universality and an efficient proof technique together with canonical examples of universal families (done in the second paper of the series [46]);
- use of this proof technique to show how some non-universal concrete families can recover universality by changing the update schedule of the system, thus extending previous results like [28, 29, 25] (done in the third paper of the series [47]).

Besides, we believe that several research directions directly connected to the notion of intrinsic universality are worth being considered. An obvious direction is to classify classical known families with respect to intrinsic universality. We expect that strong universality is very common among natural concrete families of automata networks, however we expect that deciding universality is a hard problem. Concretely, we conjecture that the following problem is undecidable: given a set of local maps in  $Q^\Delta \rightarrow Q$  decide whether the associated automata network family of bounded degree  $\Delta$  is strongly universal.

In addition, two notions of intrinsic universality are introduced in this paper, and we showed that families coming from intrinsically universal cellular automata on  $\mathbb{Z}^d$  are not strongly universal but very close to be. This raises questions about natural examples separating these different notions. Separation between universality and strong

universality is addressed in [46]. For the link with cellular automata, if we stick to local rules of bounded degree  $\Delta$ , we can ask the following questions: what are the local rules  $\lambda : Q^\Delta \rightarrow Q$  that fail to achieve intrinsic universality as cellular automaton but that does achieve strong universality when considered as an automata network family on arbitrary graphs of degree  $\Delta$ ? Conversely what are rules that achieve intrinsic universality as cellular automata but not strong universality as automata network family?

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