About non-monotony in Boolean automata networks

Mathilde Noual^{1,3}, Damien Regnault², Sylvain Sené^{2,3,*}

¹ Université de Lyon, ÉNS-Lyon, LIP, CNRS UMR 5668, 69007 Lyon, France

² Université d'Évry – Val d'Essonne, IBISC, ÉA 4526, 91000 Évry, France

 * Corresponding author: sylvain.sene@ibisc.univ-evry.fr

Abstract

This paper aims at presenting motivations and first results of a prospective theoretical study on the role of non-monotone interactions in the modelling process of biological regulation networks. Focusing on discrete models of these networks, namely, Boolean automata networks, we propose to analyse the contribution of non-monotony to the diversity and complexity in their dynamical behaviours. More precisely, in this paper, we start by detailing some motivations, both mathematical and biological, for our interest in non-monotony, and we discuss how it may account for phenomena that cannot be produced by monotony only. Then, to build some understanding in this direction, we show some preliminary results on the dynamical behaviours of some specific non-monotone Boolean automata networks called XOR circulant networks.

Keywords: Discrete dynamical systems, Boolean automata networks, non-monotony, dynamical behaviours.

1. Introduction

The introduction of Boolean automata networks by McCulloch and Pitts in [1] and Kauffman in [2, 3] initiated many developments in the study of discrete dynamical systems at the frontier of biology, mathematics and theoretical computer science. In the context of modelling biological regulation networks, the pertinence of abstract networks was deeply motivated by Hopfield and Kauffman in the respective contexts of neural and genetic networks. Among other things, Hopfield showed in [4, 5] that threshold Boolean automata networks allow to highlight the fundamental neural concepts of associative memory and learning. In [6, 7], on the basis of the breakthroughs of Jacob and Monod [8, 9], Kauffman put emphasis on the

Preprint submitted to Theoretical Computer Science

May 22, 2012

³ Institut rhône-alpin des systèmes complexes, IXXI, 69007 Lyon, France

Boolean nature of genes that are simply either actively transcribing or not. These works as well as Thomas' [10, 11, 12] placed formal approaches at the centre of the understanding of dynamical behaviours and complexity in biology. In particular, both these works claimed that theoretical frameworks would certainly allow biologists to bypass the observational knowledge which cannot, alone, lead to general conclusions. Since then, numerous theoretical studies have been carried out to acquire a better understanding of these networks, from the computational complexity standpoint [13, 14, 15, 16, 17] as well as from the standpoint of the characterisation of their dynamical behaviours [18, 19, 20, 21, 22, 23, 24, 25, 26].

In the lines of these studies and in order to supplement them, we propose in this paper to tackle the question of the role of non-monotony in Boolean automata networks. This question seems to be missing in classical literature dealing with Boolean automata networks as models of biological networks and, in particular, as models of genetic regulation networks. Indeed, on the one hand, the underlying interaction structure of Boolean models of genetic regulation networks are often represented by *signed* digraphs where vertices represent genes, and arcs, which are labelled either by a plus or a minus sign, represent directed actions of genes on one another, either activations or inhibitions. This way, a gene that tends to influence the expression of another gene is supposed to be either one of its activators or one of its inhibitors. It cannot be both. That is, it cannot act as an activator under some circumstances and act as an inhibitor under some other. This interpretation of gene regulations leads to define monotone Boolean automata networks as studied in [27, 28, 29, 30, 31, 32] and [33, 34, 35, 36, 37] from theoretical and applied points of view respectively. On the other hand, the class of linear networks has also been studied. This class contains in particular the special non-monotone networks in which all local functions are XOR functions. In [38], Cull based his study on [1, 39, 40] and developed an algebraic description of the dynamical behaviour of linear networks. In [41], Snoussi gave a characterisation of behaviours of very specific XOR networks. But the global dynamical properties of general nonmonotone networks have not yet been studied nor has the impact of nonmonotone interactions yet been examined per se.

Our recent studies on Boolean automata networks have however brought us to believe that non-monotony may be one of the main causes of singular behaviours of Boolean automata networks. Thus, this research axis seems very pertinent in the context of biological regulation networks. The present paper provides the grounds of a *prospective study* on non-monotony in networks. In this context, we develop two lines. First, with some examples, we give some insights that support the importance of non-monotony and the idea that it may be responsible for peculiar network dynamical behaviours. Second, to serve as a tangible starting point and build intuition, we present some primary results concerning a particular class of non-monotone networks called XOR circulant networks.

In Section 2, we provide general definitions and notations about Boolean automata networks that are necessary for the sequel. Section 3 details why we believe that non-monotony is in some sense at the centre of the existence of specific dynamical behaviours. Section 4 presents preliminary results concerning XOR circulant networks. In particular, it gives properties of their trajectorial behaviours by focusing on convergence times and of their asymptotic behaviours by characterising attractors. Finally, Section 5 proposes perspectives arising from this first work on non-monotony.

2. Preliminary elements on Boolean automata networks

Informally, a *Boolean automata network* involves interacting elements whose states, which either equal 0 (inactive) or 1 (active), may change over time under the influence of the states of other network elements [18, 42]. This section formalises this description by presenting the main definitions and notations which are used in this paper.

2.1. Structure and local transition functions

A Boolean automata network N of size n is composed of n elements called automata which are, by convention here, numbered from 0 to n-1. For any automaton i of $V = \{0, \ldots, n-1\}$, the set of possible states x_i of i is $\{0, 1\}$. Let us assume that the time space \mathcal{T} is discrete, i.e., $\mathcal{T} = \mathbb{N}$. A configuration of N corresponds to the allocation of a value of $\{0, 1\}$ to every automaton of N. It can thus be represented by a vector $x = (x_0, \ldots, x_{n-1}) \in \{0, 1\}^n$ and $\{0, 1\}^n$ is then the configuration space of N. Abusing language, we will denote by x(t) (resp. $x_i(t)$) the configuration of N (resp. the state of automaton i) at time step $t \in \mathcal{T}$. Given an arbitrary configuration $x \in$ $\{0, 1\}^n$, the density of x is defined as $d(x) = \frac{1}{n} \cdot |\{x_i \mid (i \in V) \land (x_i = 1)\}|$. In our context, we focus particularly on switches of automata states starting in a given network configuration. For this reason, the following notations

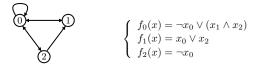


Figure 1: (left) An interaction graph of a Boolean automata network of size 3 and (right) the local transition functions of its automata.

for network configurations will be useful:

$$\forall x = (x_0, \dots, x_{n-1}) \in \{0, 1\}^n, \forall i \in V = \{0, \dots, n-1\}, \\ \overline{x}^i = (x_0, \dots, x_{i-1}, \neg x_i, x_{i+1}, \dots, x_{n-1}) \\ \text{and, } \forall W \subseteq V, \ \overline{x}^{W \cup \{i\}} = \overline{\overline{x}^W}^i.$$
(1)

Thus, in particular, $\overline{0}^i$ where $i \in V$ (resp. $\overline{0}^W$ where $W \subseteq V$) denotes the network configuration in which automaton i has state 1 (resp. all the automata belonging to W have state 1) and all other automata have state 0. The underlying interaction structure of N can be represented by a digraph G = (V, A), called the *interaction graph* of N. In this digraph, V equals the set of automata of N. $A \subseteq V \times V$ is the interaction set. For any automata $i, j \in V$, it satisfies $(j, i) \in A$ if and only if j effectively influences i, that is, in some network configurations (but not necessarily in all of them), the state of j may cause a change of states of i (see Equation 2 below). As an example, Figure 1 (left) pictures the interaction graph of a Boolean automata network of size 3, where $A = \{(0,0), (0,1), (0,2), (1,0), (2,0), (2,1)\}$. Interaction graphs specify what influences apply to each automaton of a network N. The nature of these influences are defined by the *local transition functions* $f_i : \{0,1\}^n \to \{0,1\}$ which are associated to each automaton i of N (as in Figure 1 (right)) so that:

$$\exists x \in \{0,1\}^n, \ f_i(x) \neq f_i(\overline{x}^j) \iff (j,i) \in A.$$
(2)

Thus, a Boolean automata network is entirely defined by the set of local transition functions of its automata.

2.2. Updating modes and transition graphs

To determine the possible *behaviours* of a network, it remains to be specified how automata states are updated over time. The most general point of view consists in considering all possibilities. That is, assimilating networks with state transition systems, in each configuration, $2^n - 1$ transitions are considered, one for each non-empty set of automata whose states can be updated. More precisely, $\forall W \neq \emptyset \subseteq V$, we define the update function $F_W: \{0,1\}^n \to \{0,1\}^n$ such that:

$$\forall x \in \{0,1\}^n, \forall i \in V, \ F_W(x)_i = \begin{cases} f_i(x) & \text{if } i \in W, \\ x_i & \text{otherwise.} \end{cases}$$

Then, according to the most general updating mode, the global network behaviour is given by the general transition graph $\mathcal{G}_g = (\{0,1\}^n, T_g)$ where $T_g = \{(x, F_W(x)) \mid x \in \{0,1\}^n, W \neq \emptyset \subseteq V\}$ [43, 44, 45]. In this graph which usually is a multigraph, arcs can be labelled by the set W of automata that are updated in the corresponding transition $(x, F_W(x))$. For the sake of clarity, in the examples of this paper, arcs with identical extremities are represented by a unique arc with several labels. Figure 2 (top) depicts the general transition graph of the network presented in Figure 1.

Transitions $(x, F_i(x))$ that only involve the update of one automaton $i \in V$ are called asynchronous transitions. Transitions $(x, F_W(x)), |W| > 1$ that involve the update of several are called synchronous transitions. The subgraph $\mathcal{G}_a = (\{0, 1\}^n, T_a)$ of \mathcal{G}_g whose set of arcs $T_a = \{(x, F_{\{i\}}(x)) \mid x \in \{0, 1\}^n, i \in V\}$ equals the set of asynchronous transitions of the network is called the asynchronous transition graph. This graph defines the asynchronous updating mode according to which, in each configuration, only ntransitions are considered, one for each automaton that can be updated alone. This updating mode has been widely used in studies of Thomas and his co-workers in [11, 12, 23, 29, 46, 47]. An illustration of an asynchronous transition graph is given in Figure 2 (bottom).

Because both the general and the asynchronous transition graphs are very large graphs, in some cases, to draw some intuitions, it may be necessary to restrict our attention to the transitions that are allowed under a specific deterministic updating schedule u. This amounts to considering a transition graph $\mathcal{G}_u = (\{0,1\}^n, T_u)$ which is the graph of a function $F[u] : \{0,1\}^n \to$ $\{0,1\}^n$ (*i.e.*, $T_u = \{(x, F[u](x)) \mid x \in \{0,1\}^n\}$). This function has the following form: $F[u] = F_{W_{p-1}} \circ \ldots \circ F_{W_1} \circ F_{W_0}$ where $p \in \mathbb{N}$ and $\forall k \leq$ $p, W_k \subseteq V$. It is called the global transition function associated to the updating schedule u, that updates simultaneously all automata in W_0 , then updates simultaneously all automata in $W_1 \ldots$ This second point of view has been adopted in [48, 49, 50, 51, 52, 53] following the introduction of blocksequential updating schedules by Robert in [18, 54] (see Figure 3). Section 4 is set in similar lines. It focuses on the parallel updating mode π which consists

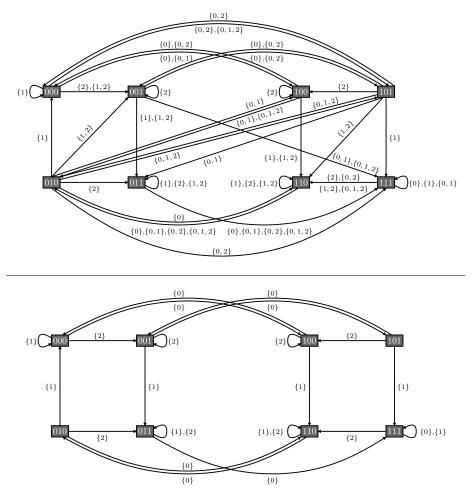


Figure 2: (top) General and (bottom) asynchronous transition graphs of the Boolean automata network of Figure 1.

in deterministically updating all network automata at once in each network configuration. In this case, the global transition function is $F[\pi] = F_V$ so that $\forall i \in V$, $F[\pi](x)_i = f_i(x)$ and the network behaviour is considered to be described by the graph of $F[\pi]$, that is, the transition graph $\mathcal{G}_{\pi} =$ $(\{0,1\}^n, T_{\pi})$ where $T_{\pi} = \{(x, F[\pi](x)) \mid x \in \{0,1\}^n\}$.

2.3. Dynamical behaviours and non-monotony

Let N be an arbitrary Boolean automata network. Consider any updating mode u among those defined above and let \mathcal{G}_u be the corresponding transi-

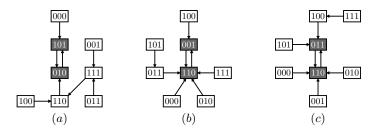


Figure 3: Transition graphs of the Boolean automata network of Figure 1 associated to (a) the parallel updating mode, (b) a block-sequential updating schedule u whose global transition function is $F[u] = F_{\{1,2\}} \circ F_{\{0\}}$ and (c) a particular block-sequential updating schedule s, called sequential, whose global transition function is $F[u] = F_{\{1\}} \circ F_{\{2\}} \circ F_{\{0\}}$. Recurrent configurations appear in grey.

tion graph. Let $x \in \{0,1\}^n$ be a configuration of N. We call trajectory of x any path in \mathcal{G}_u that starts in x. Terminal strongly connected components (*i.e.*, strongly connected components from which there are no outgoing arcs) of \mathcal{G}_u are called the *attractors* of N and constitute the asymptotic behaviours of N. Their size equals the number of configurations that they contain. Configurations that belong to an attractor are called *recurrent configurations*. Attractors of size 1 (resp. of size strictly greater than 1) are called *stable* configurations (resp. stable oscillations). When $\mathcal{G} = \mathcal{G}_u$ is the transition graph associated to a deterministic updating schedule u, stable configurations correspond to fixed points of the global transition function F[u] and stable oscillations of size p, which are rather called *limit cycles* of *period* pin this case, correspond to oriented cycles in \mathcal{G}_u . As an example, Figure 3 shows that the network of Figure 1 admits one unique attractor, a limit cycle of period 2, under any of the three deterministic updating schedules considered. The precise definition of this limit cycle, however, differs in each case. In particular, as proven in [50, 55], no configurations besides stable configurations are recurrent under the parallel updating schedule as well as under the sequential updating schedule which updates one automaton at each time step. Furthermore, Figure 2 shows that the same network admits one unique attractor, a stable oscillation of size 8, indifferently when it is subjected to the asynchronous or general updating modes.

By analogy with continuous functions, the local transition function f_i of an automaton $i \in V$ is said to be *locally monotone* in $j \in V$ if, either:

$$\forall x = (x_0, \dots, x_{n-1}) \in \{0, 1\}^n, f_i(x_0, \dots, x_{j-1}, 0, x_{j+1}, \dots, x_{n-1}) \le f_i(x_0, \dots, x_{j-1}, 1, x_{j+1}, \dots, x_{n-1})$$

$$\forall x = (x_0, \dots, x_{n-1}) \in \{0, 1\}^n, f_i(x_0, \dots, x_{j-1}, 0, x_{j+1}, \dots, x_{n-1}) \ge f_i(x_0, \dots, x_{j-1}, 1, x_{j+1}, \dots, x_{n-1}).$$

In other terms, f_i is locally monotone in j if, in the conjunctive normal form of $f_i(x)$, either only x_j appears or only $\neg x_j$ does. The function f_i is said to be locally monotone or simply monotone if it is locally monotone in all $j \in V$. It is said to be non (locally) monotone otherwise. In this latter case, there exists $j \in V$ such that in some configurations, the state of i imitates that of j and in some other configurations, on the contrary, the state of i negates that of j. When all functions f_i , $i \in V$, are monotone, the network is said to be monotone itself. Otherwise, if at least one local transition function is non-monotone, the network is said to be non-monotone. Note that we distinguish totally non-monotone networks (with only non-monotone local transition functions) from partially non-monotone networks (composed by at least one local monotone transition function).

3. Motivations

This section provides three arguments that led us to focus on non-monotony. The first one highlights the existence of non-monotone phenomena in biology whereas the last two emphasise two formal reasons about why such a study about the impact of non-monotony is of interest.

Biological view. To put forward the importance of studying non-monotony in discrete models of regulation networks, let us first recall the fundamental concept of molecular biology establishing that a gene is a portion of the DNA which is transcribed into a mRNA (the gene is then said to be expressed) that is itself translated into one or several proteins, called the *products* of that gene. Because proteins can influence the transcription and translation stages, genes have the possibility of interacting with one another through their products. Further, because the effect of a protein may depend on its concentration in the cell, genes may have different effects on one another. If gene g_j influences the expression of gene g_i via one of its protein products p, then it may do so differently according to the concentration of p in the cell. As an illustration, let us consider the infection of a bacterium *Escherichia coli* by a phage λ [56]. The genetic regulations that allow a phage λ to enter

or:

its lysogenic and lytic cycles¹ involve two genes, Cro and cl. Indeed, at high temperature [57, 58], Cro influences itself and the nature of this influence is different according to the concentration of its protein product p_{Cro} . More precisely, let us consider the model of the genetic regulation of the phage Lambda proposed in [58]. Firstly, notice that this model is an automata network evolving asynchronously which is not Boolean. Indeed, the state of Cro can take values in $\{0, 1, 2\}$ while that of cl can take values in $\{0, 1\}$. The underlying interactions in the model are the following: (i) Cro is globally inhibited by cl and also is inhibited by itself when its state equals 2; (ii) cl is inhibited by both Cro and itself. What the authors showed is that, at high temperature and whatever the state of cl is, the state of Cro goes from state 0 to state 1 (which corresponds to its basal expression), from state 1 to state 2 (which corresponds to an auto-activation of Cro because, if not, cl at state 1 should make Cro go from state 1 to state 0; more precisely, that means that the auto-activation of Cro is stronger than the inhibition coming from cl) and from state 2 to state 1 (which corresponds to an auto-inhibition of Cro as it is explained by the authors). Such a dynamical behaviour shows that the nature of the auto-interaction of Cro is twofold: it is both an auto-activation and an auto-inhibition. As a result, the only possible way to reproduce with a Boolean model the ability of Cro to present an auto-activation (a plus-signed loop that allows it to remain activated during several time steps), and an auto-inhibition (a minus-signed loop that allows it to switch its state) as it is the case in the original model is to use a nonmonotone Boolean loop on Cro. Now, supposing that Boolean automata networks are reasonable models of genetic networks, such a duality in the nature of influence of one gene g_i on the state of the same or another gene g_i corresponds precisely to the formal notion of non-monotony, specifically, that of $f_i(x)$ with respect to x_i .

Network separability. In the light of some recent developments [44, 59], the study of non-monotony in discrete networks also seems pertinent from a different, mathematical standpoint. Indeed, first, let us consider the problem of modularity in gene regulation networks which is essential in the context of biology. Modules are informally defined as independent groups of interacting genes. More precisely, they involve "biobricks" (*i.e.*, minimal sets of

¹The lysogenic cycle of a phage λ is the stage where its genome is inserted in the genome of the bacterium. Its lytic cycle is the stage where it replicates, leading *in fine* to the death of the bacterium.

genes) that own independent behaviours specific to real biological functions. Until now, the notion of modularity used in the literature relies on structural parameters [60, 61, 62]. For instance, modules are often defined simply as strongly connected components. However, although such structural definitions are natural, they can only lead to structural results, necessarily failing to reveal biobricks. In [59], a new notion of modularity is introduced for asynchronous multi-state automata networks considered as discrete models of gene regulation networks. It is supported by dynamical considerations that take into account the asymptotic behaviours of these networks. Indeed, given a network N, the method developed aims at finding a specific ordered partition² P of its automata. Such a P needs to be so that the execution of a specific composition operation (created ad hoc to adapt to the concept of attractors) applied to the recurrent configurations restricted to the elements of P, according to the total order induced by P, results in obtaining the global set of recurrent configurations of N itself (see [59] for details about the method). If such a P exists for N, then P is called a modular organisation of N and each subset composing P is called a module of N. In this context, it has been shown that any topological ordering³ on the set of strongly connected components of the underlying structure of a network N does indeed define a modular organisation of N. However, in the general case, strongly connected components are not minimal modules and thus do not allow to reveal biobricks. In some cases, they can be decomposed into smaller independent sub-modules. What is interesting is that for Boolean automata networks, except negative circuits (*i.e.*, circuits composed of an odd number of negative interactions) whose specific role is well known [11, 63] and whose intrinsic nature suffices to explain why they are not decomposable, all encountered examples of non-decomposable strongly connected components involve non-monotony.

Synchronism sensitiveness. In different lines, the importance of non-monotony can also be seen by adapting some results presented in [44]. This produces Proposition 1 which relates non-monotony to the notion of synchronism sensitiveness, which is defined below.

²An ordered partition (S_0, \ldots, S_{k-1}) of an arbitrary set S, is defined by $k \leq |S|$ nonempty ordered subsets $S_i \subset S$ such that $S = \bigoplus_{i < k} S_i$ (*i.e.*, $\forall i, j < k, i \neq j \Rightarrow S_i \cap S_j = \emptyset$ and $S = \bigcup_{i < k} S_i$).

³If G = (V, A) is a digraph, a topological ordering of G is a linear ordering of the vertices in V such that, $\forall (i, j) \in A$, i comes before j in the ordering.

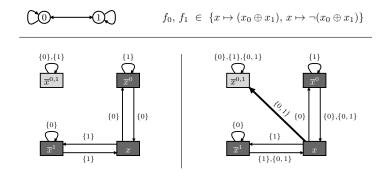


Figure 4: Top panel: Generic description of the four smallest Boolean automata networks that satisfy the conditions of Proposition 1. Bottom panels: generic (see proof of Proposition 1) (left) asynchronous and (right) general transition graphs of these networks.

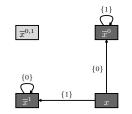
Definition 1. A Boolean automata network N is synchronism sensitive if a configuration that is recurrent in its asynchronous transition graph is not recurrent anymore in its general transition graph.

Let us add that, in the proof of Proposition 1, we make particular use of the notion of *non-sequentialisable transition* that can be derived easily from the following definition.

Definition 2. A transition $(x, F_W(x))$ is said to be sequentialisable if a series of consecutive asynchronous transitions $(x, F_{\{i\}}(x)), (F_{\{i\}}(x), F_{\{j\}} \circ F_{\{i\}}(x)), \ldots$ that starts in x and ends in $F_W(x)$ exists.

Proposition 1. The smallest Boolean automata networks that are synchonism sensitive are totally non-monotone.

Proof. Obviously, in order to be synchronism sensitive, a Boolean automata network must have at least one non-sequentialisable synchronous transition in its general transition graph. So, let us find what is the structure that a smallest network N with a non-sequentialisable synchronous transition has to verify in order to be synchronism sensitive. First, such a network needs to have more than one automaton and if it has size 2, then, to have a non-sequentialisable synchronous transition, its general transition graph needs to contain a subgraph (with asynchronous transitions only) of the following form:



where $\overline{x}^{i,j} = \overline{x}^{\{i,j\}} = \overline{\overline{x}^{i,j}}$ (see Equation 1). This subgraph is the smallest that is necessary for the general transition graph to contain a nonsequentialisable synchronous transition, which is $(x, \overline{x}^{i,j})$ in this case. Moreover, to guarantee synchronism sensitivity, since fixed points are conserved whatever the updating mode is, the synchronous transition $(x, \overline{x}^{i,j})$ must go out from a set of configurations belonging to an asynchronous stable oscillation. Now, the only way to create an asynchronous stable oscillation validating the presence of the asynchronous subgraph drawn above is to add transitions (\overline{x}^i, x) and (\overline{x}^j, x) . On this basis, in order to create synchronism sensitivity, configuration $\overline{x}^{i,j}$ must be a fixed point of N. Indeed, if not, $\overline{x}^{i,j}$ is a predecessor of the limit cycle and adding synchronism will maintain every asynchronous recurrent configurations. Thus, since $\overline{x}^{i,j}$ is a fixed point of N, adding transition $(x, \overline{x}^{i,j})$ makes $\overline{x}^{i,j}$ become the only attractor of N with respect to the general updating mode. Then, the general transition graph of N must have the form of that pictured in the bottom right panel of Figure 4 (note that the bottom left panel of this figure illustrates the asynchronous transition graph of such a N to compare). Consequently, only two functions f_0 are possible. If in configuration x above, $x_0 = 1$, then, $f_0(x): x \mapsto x_0 \oplus x_1$ where \oplus denotes the XOR connector⁴. If in configuration x above, $x_0 = 0$, then $f_0(x) : x \mapsto \neg(x_0 \oplus x_1)$. The function f_1 is defined similarly. In conclusion, there are four smallest networks satisfying the properties of Proposition 1. They have size 2 and their interactions graph equal the graph pictured in the top panel of Figure 4. Their two local interaction functions f_0 and f_1 either equal $x \mapsto x_0 \oplus x_1$ or $x \mapsto \neg(x_0 \oplus x_1)$.

The reasons evoked in this section that led us to focus on non-monotony in automata networks emphasise the apparent importance of non-monotone functions. In the next section, to initiate an analysis of the behaviours of general non-monotone networks and develop some intuition in this direction, we focus on a specific class of non-monotone networks, namely XOR circulant networks, and study some of their dynamical properties.

 ${}^{4}\forall a, b \in \{0, 1\}, a \oplus b = (a \land \neg b) \lor (\neg a \land b).$

4. XOR circulant networks

In this section, we present some results on the trajectorial and asymptotic dynamical behaviours of XOR circulant networks. Let us briefly say that the choice of these specific networks comes directly from Proposition 1 and from the fact that they represent a class of non-monotone Boolean automata networks not too large which gets all the necessary properties allowing them to present complex dynamical behaviours (see further). Before the results, let us first introduce some definitions and preliminary properties in relation to these networks.

4.1. Definitions and basic properties

A circulant matrix C is a matrix of order n whose i^{th} row vector C_i (i < n) is the right-cyclic permutation with offset i of its first row vector C_0 so that C has the following form:

$$C = \begin{pmatrix} c_0 & c_1 & c_2 & \dots & c_{n-1} \\ c_{n-1} & c_0 & c_1 & \dots & c_{n-2} \\ c_{n-2} & c_{n-1} & c_0 & \dots & c_{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_1 & c_2 & c_3 & \dots & c_0 \end{pmatrix}.$$

For any integer $k \geq 2$, a k-XOR *circulant network* of size $n \geq k$ is a Boolean automata network with n automata that can be numbered so that the following four properties are satisfied: (i) the adjacency matrix C of the network interaction graph G = (V, A) (*i.e.*, the $n \times n$ matrix C defined by $\forall i, j \in V, C_{i,j} = 1 \iff (j, i) \in A$), called the *interaction matrix* for short, is a circulant matrix, (ii) each row C_i , $i \in V$, of this matrix contains exactly k non-null coefficients (*i.e.*, $\forall i \in V, \sum_{j \in V} C_{i,j} = deg_G^-(i) = k$), (*iii*) $C_{0,n-1} = c_{n-1} = 1$ and (*iv*) the local transition function f_i of any automatom $i \in V$ is a XOR function:

$$\forall x \in \{0,1\}^n, \ f_i(x) = \bigoplus_{j \in V} \mathcal{C}_{i,j} \cdot x_j = \sum_{j \in V} \mathcal{C}_{i,j} \cdot x_j \ [2],$$

where, for any integers a and b, a [b] stands for a (mod b). In the sequel, for the sake of simplicity, XOR circulant networks are considered to be subjected to the *parallel updating mode* so that if $x = x(t) \in \{0,1\}^n$ is the network configuration at time step $t \in \mathcal{T}$, then the network configuration at time step t+1 equals $x(t+1) = F(x) = \mathcal{C} \cdot x$ (where operations are supposed to be taken

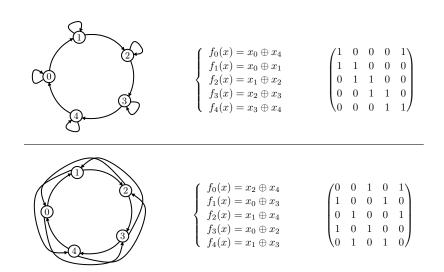


Figure 5: Interaction graphs, local transition functions and interaction matrices of two 2-XOR circulant networks of sizes 5.

modulo 2). Notice that F is as a consequence a linear function [38, 40, 64]. Thus, a XOR circulant network is completely defined by its interaction graph G = (V, A) or by its interaction matrix C. Figure 5 pictures two examples of 2-XOR circulant networks of size 5. Let us note that one of the four networks satisfying Proposition 1 and defined in Figure 4 is also a 2-XOR circulant network of size 2.

Let us note that by point (iii) in their definitions, k-XOR circulant networks have Hamiltonian circuits underlying their structures. When automata are numbered as suggested in this definition, these circuits are composed of the set of arcs $\{(i, i + 1 \ [n]) \mid i \in V\} \subseteq A$. More generally, it can be shown that each non-null coefficient $c_j = C_{0,j}$ of a circulant interaction matrix C induces gcd(n, j) independent circuits of length n/gcd(n, j) in the interaction graph G of the corresponding network. Now, it has been shown that to have several stable configurations and/or stable oscillations, Boolean automata networks need to have circuits underlying their interaction graphs [11, 47, 63]. Thus, the presence of circuits underlying the structures of k-XOR circulant networks increases significantly their chances to have interesting, non-trivial dynamical behaviours, which will be shown in the sequel.

Any k-XOR circulant network N can be seen in terms of *cellular automata*. Indeed, if N has size n and interaction graph G = (V, A), it can be modelled by the finite one-dimensional cellular automaton that has n cells assimilated to the n automata of N and that satisfies what follows. The *neighbour*-

hood \mathcal{N} of a cell $i \in V$ equals the in-neighbourhood of automaton i in N: $\mathcal{N} = \{j \in V \mid (j,i) \in A\}$. The local rule $\gamma : \{0,1\}^{|\mathcal{N}|} \to \{0,1\}$ of the cellular automaton is defined similarly to the local transition functions of N: $\gamma((x_{\ell})_{\ell \in \mathcal{N}}) = \bigoplus_{\ell \in \mathcal{N}} x_{\ell}$. In the sequel, we use this formalisation to exploit tools drawn from the theory of cellular automata. Thus, if $x = x(0) \in \{0, 1\}^n$ is an initial configuration of N, we consider the corresponding *space-time diagram*, that is, the grid of $\{0, 1\}^n \times \mathcal{T}$ whose line $t \in \mathcal{T}$ represents x(t), *i.e.*, the configuration of N at time step t. The trace of cell or automaton $i \in V$ then corresponds to column i of this grid, that is, to the sequence $(x_i(t))_{t \in \mathcal{T}}$. Also, for an arbitrary configuration $x \in \{0,1\}^n$ and an automaton $i \in V$, $R_i(x)$ denotes the configuration that satisfies $\forall j \in V, R_i(x)_j = x_{2i-j} [n]$. It is called the *reflection of* x with respect to i. We write \widetilde{N} to denote the reflection of N, that is, the k-XOR circulant network whose interaction matrix is ${}^{t}\mathcal{C}$. In the sequel, by default, $\mathcal{N}^{-}(i)$ (resp. $\mathcal{N}^{+}(i)$) denotes the *in*neighbourhood (resp. the out-neighbourhood) of automaton i in N and $\mathcal{N}^{-}(i)$ (resp. $\widetilde{\mathcal{N}}^+(i)$) denotes its in-neighbourhood (resp. its out-neighbourhood) in \widetilde{N} . This way, for any two automata $i, j \in V, j \in \mathcal{N}^{-}(i) \iff j \in \widetilde{\mathcal{N}}^{+}(i)$. The global transition function of \widetilde{N} is denoted by \widetilde{F} if that of N is denoted by F. Notice that F represents the reflected global transition function of N. One last convention that is used throughout the sequel is the following. By default, unless N is the reflection of another k-xor circulant network that was introduced before, its automata are supposed to be numbered as suggested above in the definition of k-XOR circulant networks so that $c_{n-1} = \mathcal{C}_{0,n-1} = 1$. This way, $\{(i, i+1 \ [n]) \mid i \in V\} \subseteq A$ defines a Hamiltonian circuit in the structure of N and $\{(i+1 \ [n], i) \mid i \in V\} \subseteq A$ defines a Hamiltonian circuit in the structure of its reflection N.

To end this paragraph, we list some basic properties of XOR circulant networks that follow directly from the definitions of XOR functions and circular matrices:

Proposition 2.

1. The number of k-XOR circulant networks of size n equals $\binom{k-1}{n-1}$.

Any k-XOR circulant network of size n satisfies the following properties:

- 2. Configuration $(0, \ldots, 0)$ is a stable configuration.
- 3. Configuration (1, ..., 1) is a predecessor of (0, ..., 0) if k is even or a stable configuration if k is odd.
- 4. The trajectory of a configuration x is isomorphic to that of any configuration y which is a circular permutation of x.

4.2. Results

In order not to burden the reading in the sequel, note that, unless it is mentioned, the automata are always taken modulo the size n of the network considered.

4.2.1. General k-XOR circulant networks

First, in this paragraph, we concentrate on general k-XOR circulant networks and exploit the cellular automata formalisation presented above to derive some features of the dynamical behaviours of these networks.

Lemma 1. Let N be a k-XOR circulant network of size n with automata set V and reflected global transition function \widetilde{F} . For any automaton $i \in V$, let $M_i(t), t \in \mathcal{T}$, denote the set of automata which have state 1 in configuration $\widetilde{F}^t(\overline{0}^i)$. Then, $\forall x(0) \in \{0,1\}^n, \forall t \in \mathcal{T}, x_i(t) = \bigoplus_{j \in M_i(t)} x_j(0)$.

Proof. We prove Lemma 1 by induction on $t \in \mathcal{T}$.

For t = 0, $M_i(0) = \{i\}$ holds by definition of configuration $\overline{0}^i$. Thus, $\forall x(0) \in \{0,1\}^n$, $x_i(0) = \bigoplus_{j \in M_i(0)} x_j(0)$.

Now, suppose that $\forall x(0) \in \{0,1\}^n$, $x_i(t) = \bigoplus_{j \in M_i(t)} x_j(0)$ and consider the initial configuration $y(0) \in \{0,1\}^n$.

Since $y(t+1) = \tilde{F}^{t+1}(y(0)) = \tilde{F}^t(y(1))$, applying the induction hypothesis to configuration x(0) = y(1) yields:

$$y_i(t+1) = \bigoplus_{j \in M_i(t)} y_j(1).$$

By definition, $\forall j \in V$, $y_j(1) = f_j(y(0)) = \bigoplus_{\ell \in \mathcal{N}^-(j)} y_\ell(0) = \bigoplus_{\ell \in \widetilde{\mathcal{N}}^+(j)} y_\ell(0)$. Thus, with the commutativity and associativity of the \oplus operator, we can derive that:

$$y_i(t+1) = \bigoplus_{j \in M_i(t)} \left(\bigoplus_{\ell \in \widetilde{\mathcal{N}}^+(j)} y_\ell(0) \right)$$
$$= \bigoplus_{\substack{\{\ell \text{ s.t. } |\widetilde{\mathcal{N}}^-(\ell) \cap M_i(t)| \equiv 1 \ [2]\}}} y_\ell(0).$$

Now, let us remark that $\forall t \in \mathcal{T}$, $\widetilde{F}(\overline{0}^{M_i(t)}) = \overline{0}^{M_i(t+1)}$ by definition. Then, $\forall \ell \in V, \overline{0}_{\ell}^{M_i(t+1)} = 1$ if and only if $|\widetilde{\mathcal{N}}^-(\ell) \cap M_i(t)| \equiv 1$ [2]. From this follows $y_i(t+1) = \bigoplus_{j \in M_i(t+1)} y_j(0)$ and then $\forall t \in \mathcal{T}, x_i(t) = \bigoplus_{j \in M_i(t)} x_j(0)$. \Box **Lemma 2.** Let N be a k-XOR circulant network of size n with automata set V and global transition function F. For any automaton $i \in V$, and for any configuration $x \in \{0,1\}^n$, it holds that $\widetilde{F}(R_i(x)) = R_i(F(x))$.

Proof. For any $j \in V$, the following holds:

$$\widetilde{F}(R_i(x))_j = \bigoplus_{\ell \in \widetilde{\mathcal{N}}^-(j)} (R_i(x))_\ell = \bigoplus_{\ell \in \widetilde{\mathcal{N}}^-(j)} x_{2i-\ell}$$
$$= \bigoplus_{\substack{\{\ell \text{ s.t. } 2i-\ell \in \widetilde{\mathcal{N}}^-(j)\}}} x_\ell$$
$$= \bigoplus_{\substack{\{\ell \text{ s.t. } j \in \mathcal{N}^-(2i-\ell)\}}} x_\ell.$$

If $j \in \mathcal{N}^{-}(2i-\ell)$, then all automata $l, l' \in V$ of N such that $l-l' = j-(2i-\ell)$ are such that $l \in \mathcal{N}^{-}(l')$. In particular, if automaton $j \in \mathcal{N}^{-}(2i-\ell)$, then $\ell \in \mathcal{N}^{-}(2i-j)$. Hence:

$$\bigoplus_{\substack{\{\ell \text{ s.t. } j \in \mathcal{N}^-(2i-\ell)\}}} x_\ell = \bigoplus_{\substack{\ell \in \mathcal{N}^-(2i-j)}} x_\ell$$
$$= F(x)_{2i-j}$$
$$= (R_i(F(x)))_j,$$

and Lemma 2 follows.

Proposition 3. Let N be a k-XOR circulant network of size n with automata set V and global transition function F. For any automaton $i \in V$ and for the initial configuration $x(0) = \overline{0}^i$, it holds that $\forall t \in \mathcal{T}, \widetilde{F}^t(x(0)) = R_i(x(t))$.

Proof. Proposition 3 is proven by induction on $t \in \mathcal{T}$. Let t = 0. Property $\widetilde{F}^t(x(0)) = R_i(x(t))$ is true because $x(0) = \overline{0}^i$. Suppose that it is true for $t \in \mathcal{T}$. Then, we have $\widetilde{F}^{t+1}(x(0)) = \widetilde{F}(\widetilde{F}^t(x(0))) = \widetilde{F}(R_i(x(t)))$. By Lemma 2, $\widetilde{F}(R_i(x(t)) = R_i(F(x(t)) = R_i(x(t+1)))$, which is the expected result.

Remark that this result is due to the fact that F and \tilde{F} are the global transition functions of two reflected k-XOR circulant networks that are isomorphic by definition (see Figure 6). Proposition 3 implies that, for any automaton $i \in V$, the space-time diagram of $(\overline{0}^i(t))_{t\in\mathcal{T}}$ is the reflected space-time diagram of $(\overline{0}^{M_i(t)})_{t\in\mathcal{T}}$ with respect to i and is related to the trace of automaton i. Thus, the space-time diagrams of configurations of density $\frac{1}{n}$ carry information on the global behaviours of N. We examine further these properties in the following results. **Proposition 4.** Let N be a k-XOR circulant network of size n with automata set V and global transition function F. The maximum convergence time, i.e., the maximal transient trajectory length, is reached by configurations of density $\frac{1}{n}$. Moreover, let p_* be the period of the attractors reached by configurations of density $\frac{1}{n}$. Then, for any configuration x of N, the period of its attractor (i.e., of the attractor that is reached by the network when it is initially in configuration x) divides p_* .

Proof. Since all configurations of density $\frac{1}{n}$ are cyclic permutations of one another, by Proposition 2.4 they all have isomorphic trajectories so that they all hit their limit set at the same time t_* and they all have the same period p_* . Now, consider configuration x and automaton i. By Proposition 3, the space-time diagram of $(\overline{0}^{M_i(t)})_{t\in\mathcal{T}}$ is the reflected space-time diagram of $(\overline{0}^i(t))_{t\in\mathcal{T}}$ with respect to i. Thus, the space-time diagram of $(\overline{0}^{M_i(t)})_{t\in\mathcal{T}}$ hits its limit set at time t_* and its period is p_* . This means that, $\forall i \in N$, the trace of automaton i has period p_* and hits its limit before t_* . Thus, the trajectory of x reaches its limit set before t_* and its period divides p_* . \Box

4.2.2. 2-XOR circulant networks

Let us now concentrate on 2-XOR circulant networks of arbitrary size nand pay particular attention to the space-time diagrams of configurations of density $\frac{1}{n}$. We define the *interaction-step* of such a network N as the smallest integer $s \neq 1 < n$ such that $\forall i \in V$, $(i, i + s) \in A$. As illustrated in Figure 6 (a) and (b), when s = 0 the space-time diagram is the Sierpinski triangle. For other values of s, space-time diagrams seem like deformed Sierpinski triangles. From these observations results the following lemma.

Lemma 3. Let N be a 2-XOR circulant network of size n with interactionstep s = 0. The following holds:

$$\forall i \in V, \forall q \in \mathbb{N}, x_i(2^q) = x_{(i-2^q)}(0) \oplus x_i(0).$$

Proof. Lemma 3 is proven by induction on q.

Let $i \in V$ be an arbitrary automaton and let q equal 1 initially. Then, obviously, the following is true:

$$\begin{aligned} x_i(2) &= x_{(i-1)}(1) \oplus x_i(1) \\ &= x_{(i-2)}(0) \oplus x_{(i-1)}(0) \oplus x_{(i-1)}(0) \oplus x_i(0) \\ &= x_{(i-2)}(0) \oplus x_i(0), \end{aligned}$$

and the basis of the induction holds.

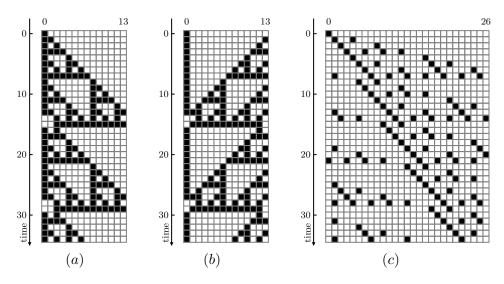


Figure 6: Space-time diagrams (a) of a 2-XOR circulant network of size 14 and interactionstep s = 0 (see Section 4.2.2), (b) of its reflected network and (c) of another 2-XOR circulant network of size 27 and interaction-step 4.

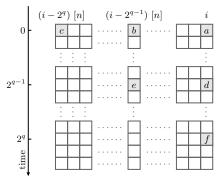


Figure 7: Space-time diagram of an arbitrary 2-xor circulant network of size n and interaction-step s = 0.

Now, let us assume as induction hypothesis that $x_i(2^q) = x_{(i-2^q)}(0) \oplus x_i(0)$ is true for $q \in \mathbb{N}$. In the sequel, we pay particular attention to states

$$a = x_i(0), \quad b = x_{(i-2^{q-1})}(0), \quad c = x_{(i-2^q)}(0), \quad d = x_i(2^{q-1}),$$

 $e = x_{(i-2^{q-1})}(2^{q-1}) \quad \text{and} \quad f = x_i(2^q),$

as illustrated in Figure 7.

Then, for q + 1, according to the induction hypothesis, we have:

$$d = a \oplus b, \quad e = b \oplus c \quad \text{and} \quad f = d \oplus e$$

Then, we derive that:

$$f = d \oplus e = (a \oplus b) \oplus (b \oplus c) = a \oplus c.$$

As a result, we can write:

$$\forall i \in V, \forall q \in \mathcal{N}, \ x_i(2^q) = x_i(0) \oplus x_{(i-2^q)}(0),$$

which is the expected result.

We will use this lemma to analyse 2-XOR circulant networks of size $n = 2^p$, $p \in \mathbb{N}^*$, and interaction step s = 0.

4.2.3. 2-XOR circulant networks of sizes powers of 2

In this paragraph, we focus on 2-XOR circulant networks of sizes $n = 2^p$, where $p \in \mathbb{N}^*$. Let $x = (x_0, \ldots, x_{n-1}) \in \{0, 1\}^n$ be a configuration of such a network N. We can see x as the concatenation of two vectors of sizes $\frac{n}{2}$ such that x = (x', x''), where $x' = (x_0, \ldots, x_{\frac{n}{2}-1})$ and $x'' = (x_{\frac{n}{2}}, \ldots, x_{n-1})$ are called *semi-configurations* of x. The *repetition degree* $\delta_r(x)$ of x is then defined as:

$$\delta_r(x = (x', x'')) = \begin{cases} 0 & \text{if } x' \neq x'', \\ \delta & \text{if } (x' = x'') \land (\delta_r(x') = \delta - 1). \end{cases}$$

Notice that if x = (x', x'), x is said to be a repeated configuration and that, in the worst case (*i.e.*, when the repetition degree $\delta_r(x) = \log_2(n)$ is maximal), the time complexity of the computation of the repetition degree of any configuration x equals n.

Proposition 5 below characterises the dynamical behaviours of repeated configurations $x \in \{0,1\}^n$ of repetition degree $\delta_r(x) \ge \log_2(n) - 1$ in arbitrary 2-XOR circulant networks of size $n = 2^p$, $p \in \mathbb{N}^*$.

Proposition 5. Let N be a 2-XOR circulant network of size $n = 2^p$, $p \in \mathbb{N}^*$, and interaction-step s. Configurations $x \in \{0,1\}^n$ of repetition degree $\delta_r(x) \ge \log_2(n) - 1$ converge towards $(0, \ldots, 0)$ in no more than 2 time steps.

Proof. First, notice that because N is a 2-XOR circulant network of size $n = 2^p$, $p \in \mathbb{N}^*$, there exist only 4 repeated configurations of degree no smaller than $\log_2(n) - 1$, that is, $(0, 1, \ldots, 0, 1)$, its dual $(1, 0, \ldots, 1, 0)$ and $(1, \ldots, 1)$ and its dual $(0, \ldots, 0)$. Let us consider the two distinct parities of s independently. Also, let $t \in \mathcal{T}$ and let x(t) be either $(0, 1, \ldots, 0, 1)$ or $(1, 0, \ldots, 1, 0)$.

1. If s is even, then, by hypothesis on x(t):

$$\forall i \in V, \ x_{(i+s)}(t+1) = x_i(t) \oplus x_{(i+s-1)}(t) = 1.$$

2. If s is odd, then, by hypothesis on x(t):

$$\forall i \in V, \ x_{(i+s)}(t+1) = x_i(t) \oplus x_{(i+s-1)}(t) = 0.$$

This, together with Propositions 2.2 and 2.3, yields the expected result. \Box

From now on, we restrict the study to 2-XOR circulant networks of sizes $n = 2^p$, $p \in \mathbb{N}^*$, and interaction-steps s = 0. We show that such networks necessarily converge towards configuration $(0, \ldots, 0)$ in no more than n time steps and that initial configurations with an odd number of 1 converge in exactly n steps.

Theorem 1. Let N be a 2-XOR circulant network of size $n = 2^p$, $p \in \mathbb{N}^*$, and interaction-step 0. Any configuration x converges to the stable configuration $(0, \ldots, 0)$ in no more than n time steps.

Proof. Since $n = 2^p$, by Lemma 3, we directly draw:

$$\forall i \in V, x_i(n) = x_i(0) \oplus x_{i+n}(0) = x_i(0) \oplus x_i(0) = 0.$$

This allows to conclude that any configuration x converges to the stable configuration $(0, \ldots, 0)$ in no more than n time steps.

Now, let us consider the configurations for which the convergence time is maximal.

Lemma 4. Let N and N' be two 2-XOR circulant networks of respective sizes $n = 2^{p+1}$ and $n' = 2^p$, $p \in \mathbb{N}^*$, and interaction-steps 0. Let x' be a configuration of size 2^p and x = (x', x') be a repeated configuration of size 2^{p+1} . Then, for any $t \in \mathcal{T}$, x(t) = (x'(t), x'(t)).

Proof. Considering an arbitrary repeated configuration x of N, by induction on t, we show that $\forall t \in \mathcal{T}$, x(t) = (x'(t), x'(t)). Let us denote by G' = (V', A') the interaction graph of N'.

By hypothesis, the proposition is true for t = 0.

Now, consider that x(t) = (x'(t), x'(t)) for $t \in \mathcal{T}$ and that

$$\forall i \in V, \ x_i(t+1) = x_{(i-1)}(t) \oplus x_i(t).$$

Since x(t) is a repeated configuration, we have:

$$\forall i \in V, \ x_i(t+1) = x_{(i-1)}(t) \oplus x_i(t)$$

= $x_{(i-1+2^p)}(t) \oplus x_{(i+2^p)}(t)$
= $x_{(i+2^p)}(t+1).$

Thus, x(t+1) is also repeated and it satisfies:

$$\forall i \in V', x_i(t+1) = x_{(i-1) \ [n']}(t) \oplus x_i(t)$$

= $x'_{(i-1) \ [n']}(t) \oplus x'_i(t)$
= $x'_i(t+1).$

As a result, it holds that x(t+1) = (x'(t+1), x'(t+1)).

Proposition 6. Let N be a 2-XOR circulant network of size $n = 2^p$, $p \in \mathbb{N}^*$, and interaction-step 0. Any configuration x such that $n \cdot d(x) \equiv 1$ [2] (with an odd number of 1s) converges in n time steps exactly.

Proof. Proposition 6 is proven by induction on p.

If p = 1, according to Propositions 2.3 and 5, configurations of repetition degree $\log_2(n)-1$ are proven to converge in 2 time steps. Thus, Proposition 6 holds for p = 1.

Suppose that for p = q, any configuration x such that $2^q \cdot d(x) \equiv 1$ [2] converges in 2^q time steps.

Now, suppose that p = q + 1 and consider a 2-xor circulant network N of size $n = 2^{q+1}$ and interaction-step 0. Let x be a configuration of size 2^{q+1} such that $n \cdot d(x) \equiv 1$ [2]. We show that after 2^q time steps:

1. $x(2^q)$ is a repeated configuration of the form $x(2^q) = (x'(2^q), x'(2^q))$. By Lemma 3, $\forall i \in \{0, ..., 2^q - 1\}, x_i(2^q) = x_i(0) \oplus x_{(i+2^q)}(0)$. Hence:

$$\forall i \in \{0, \dots, 2^q - 1\},\ x_i(2^q) = x_{(i+2^{q+1})}(0) \oplus x_{(i+2^q)}(0) = x_{(i+2^q)}(2^q).$$

2. x' has an odd number of 1s. By Lemma 3 and the property above, since $\forall i \in \{0, \ldots 2^q - 1\}, x'_i(2^q) = x_i(2^q) = x_i(0) + x_{(i+2^q)}(0)$, each automaton of x(0) influences exactly one automaton of x'. If $x'_i(2^q) = 0$, then the states of both the automata of x(0) that influence $x'_i(2^q)$ must have the same parity. If $x'_i(2^q) = 1$ then the states of both the automata of x(0) that influence $x'_i(2^q)$ must have different parities. Since there is an odd number of 1s in x(0), there is an odd number of 1s in $x'(2^q)$.

By Lemma 4, $x(2^q)$ behaves exactly like $x'(2^q)$. By the induction hypothesis, x' converges in exactly 2^q time steps. Thus x converges in exactly $n = 2^{q+1}$ time steps.

5. Conclusion and perspectives

With this study, we have endeavoured to show that non-monotony is an interesting concept per se, despite the lack of specific attention it has received so far. On the one hand, to serve as a stepping-stone and acquire some initial intuitions in this domain, we have considered a special family of non-monotone Boolean automata networks that we named XOR circulant networks. In particular, we have focused on the trajectorial and asymptotic behaviours of these networks, considered their convergence times and characterised their attractors. Globally, this preliminary formal analysis revealed that simple non-monotone networks can exhibit non-trivial, engaging properties. On the other hand, more generally and informally, we also have put forward several arguments to support the idea that work needs to be done to build a better understanding of the role of non-monotony in the behaviours of automata networks. In these lines, we have mentioned that studies in this context could find concrete and relevant applications in biology and in particular in the modelling of genetic regulation networks by automata networks. In addition, we have given two theoretical arguments in favour of our insights by which non-monotony could be responsible for singular network behaviours. First, exploiting [59], we have argued that non-monotony may be responsible for the strongly connected components of networks being non-separable, minimal functional modules. Second, in Proposition 1, with the state transition systems formalism, we have considered "synchronism sensitivity", that is the property of Boolean automata networks to display significant behavioural changes when synchronism is added to their automata state updates. And in this context, we have shown that the smallest synchronism sensitive Boolean automata networks are also non-monotone.

The issues presented in this paper open many research directions that could help develop a better understanding of the precise role of non-monotony in formal automata networks and, *a fortiori*, in real biological regulation networks. One of these perspectives consists in identifying the relations that exist between monotone and non-monotone Boolean automata networks. In [44], some preliminary results are derived on synchronism sensitivity. In particular it is shown that this property requires specific circuits

underlying the networks structures. Also, monotone examples of synchronism sensitive networks are given. The interesting point is that all of them involve linear monotone codings of non-monotony, which allows to build monotone Boolean automata networks having similar dynamical behaviours, which means monotone networks that are also synchronism sensitive. With Proposition 1, this naturally raises the question of whether non-monotony (taken in a more general sense than what we did formally above) can account in a certain way for the synchronism sensitivity in arbitrary monotone and non-monotone networks. Thus, Proposition 1 together with the work presented in [44] call for further researches in this direction. With sufficient knowledge in this context, we then hope to move on to the subject of modularity as developed in [59] and work on establishing the exact nonseparability conditions of strongly connected networks. In this context, the first important questions that need to be addressed are: "Except negative circuits, does there exist monotone strongly connected networks that are separable into functional modules?" and "How does non-monotony relate to the non-separability of non-monotone networks?". The relevance of these questions lies in that their answers will help understand modularity in biological regulation networks, which is a central issue in present biological research frameworks such as synthetic biology. Eventually, further analyses also need to be done on the dynamical behaviours of XOR circulant networks. Indeed, we believe that these networks constitute very promising instances of non-monotone networks because of their apparent simplicity and because, since they involve underlying structural circuits, their dynamical behaviours are potentially diverse and complex. Thus, pursuing in this direction, we hope to obtain generalisations of the results that figure above concerning the parallel updating mode by relaxing structural constraints step by step. Also, another interesting perspective in this framework is to consider XOR circulant networks as state transition systems, under the asynchronous and general updating modes. This perspective is motivated in particular by the fact that, according to Proposition 1, the smallest synchronism sensitive networks are either XOR circulant networks of size 2 and interaction-step 0, or networks that have the same structures as these and comparable nonmonotone interactions.

6. Acknowledgements

We thank Florian Rabin for his relevant comments and are indebted to the Agence nationale de la recherche and the Réseau national des systèmes *complexes* that have respectively supported this work through the projects Synbiotic (ANR 2010 BLAN 030701) and Météding (RNSC AI10/11-L03908).

References

- [1] W. S. McCulloch, W. Pitts, A logical calculus of the ideas immanent in nervous activity, Journal of Mathematical Biophysics 5 (1943) 115–133.
- [2] S. A. Kauffman, Metabolic stability and epigenesis in randomly constructed genetic nets, Journal of Theoretical Biology 22 (1969) 437–467.
- [3] S. A. Kauffman, Homeostasis and differentiation in random genetic control networks, Nature 224 (1969) 177–178.
- [4] J. J. Hopfield, Neural networks and physical systems with emergent collective computational abilities, Proceedings of the National Academy of Sciences of the USA 79 (1982) 2554–2558.
- [5] J. J. Hopfield, Neurons with graded response have collective computational properties like those of two-state neurons, Proceedings of the National Academy of Sciences of the USA 81 (1984) 3088–3092.
- [6] S. A. Kauffman, Current topics in developmental biology, Vol. 6, Elsevier, 1971, Ch. Gene regulation networks: a theory for their global structures and behaviors, pp. 145–181.
- [7] S. A. Kauffman, The origins of order, Oxford University Press, 1993.
- [8] F. Jacob, J. Monod, Genetic regulatory mechanisms in the synthesis of proteins, Journal of Molecular Biology 3 (1961) 318–356.
- [9] F. Jacob, J. Monod, On the regulation of gene activity, Cold Spring Harbor Symposia on Quantitative Biology 26 (1961) 193–211.
- [10] R. Thomas, Boolean formalisation of genetic control circuits, Journal of Theoretical Biology 42 (1973) 563–585.
- [11] R. Thomas, On the relation between the logical structure of systems and their ability to generate multiple steady states or sustained oscillations, in: Numerical methods in the study of critical phenomena, Vol. 9 of Springer Series in Synergetics, Springer, 1981, pp. 180–193.
- [12] R. Thomas, Regulatory networks seen as asynchronous automata: a logical description, Journal of Theoretical Biology 153 (1991) 1–23.

- [13] P. Floréen, P. Orponen, On the computational complexity of analyzing Hopfield nets, Complex Systems 3 (1989) 577–587.
- [14] M. Cosnard, P. Koiran, H. Paugam-Moisy, Complexity issues in neural network computations, in: Proceedings of LATIN, Vol. 583 of Lecture Notes in Computer Science, Springer, 1992, pp. 530–544.
- [15] P. Koiran, Puissance de calcul des réseaux de neurones artificiels, Ph.D. thesis, École normale supérieure de Lyon (1993).
- [16] P. Orponen, Computing with truly asynchronous threshold logic networks, Theoretical Computer Science 174 (1997) 123–136.
- [17] A. Gajardo, A. Moreira, E. Goles, Complexity of Langton's ant, Discrete Applied Mathematics 117 (2002) 41–50.
- [18] F. Robert, Discrete iterations: a metric study, Vol. 6 of Springer Series in Computational Mathematics, Springer, 1986.
- [19] E. Goles, J. Olivos, Comportement périodique des fonctions à seuil binaires et applications, Discrete Applied Mathematics 3 (1981) 93– 105.
- [20] E. Goles, Neural and automata networks: dynamical behaviour and applications, Mathematics and its applications, Kluwer Academic Publishers, 1990.
- [21] J. Aracena, J. Demongeot, E. Goles, Fixed points and maximal independent sets in AND-OR networks, Discrete Applied Mathematics 138 (2004) 277–288.
- [22] J. Aracena, J. Demongeot, E. Goles, On limit cycles of monotone functions with symmetric connection graph, Theoretical Computer Science 322 (2004) 237–244.
- [23] É. Remy, P. Ruet, D. Thieffry, Graphic requirements for multistability and attractive cycles in a Boolean dynamical framework, Advances in Applied Mathematics 41 (2008) 335–350.
- [24] J. Demongeot, E. Goles, M. Morvan, M. Noual, S. Sené, Attraction basins as gauges of robustness against boundary conditions in biological complex systems, PLoS One 5 (2010) e11793.
- [25] J. Demongeot, M. Noual, S. Sené, Combinatorics of Boolean automata circuits dynamics, Discrete Applied Mathematics 160 (2012) 398–415.

- [26] A. Richard, Local negative circuits and fixed points in non-expansive Boolean networks, Discrete Applied Mathematics 159 (2011) 1085– 1093.
- [27] E. Goles-Chacc, F. Fogelman-Soulie, D. Pellegrin, Decreasing energy functions as a tool for studying threshold networks, Discrete Applied Mathematics 12 (1985) 261–277.
- [28] M. Cosnard, E. Goles, Discrete state neural networks and energies, Neural Networks 10 (1997) 327–334.
- [29] É. Remy, B. Mossé, C. Chaouiya, D. Thieffry, A description of dynamical graphs associated to elementary regulatory circuits, Bioinformatics 19 (2003) ii172–ii178.
- [30] C. Chaouiya, É. Remy, P. Ruet, D. Thieffry, Qualitative modelling of genetic networks: from logical regulatory graphs to standard Petri nets, in: Proceedings of Petri Nets, Vol. 3099 of Lecture Notes in Computer Science, Springer, 2004, pp. 137–156.
- [31] O. Colón-Reyes, R. Laubenbacher, B. Pareigis, Boolean monomial dynamical systems, Annals of Combinatorics 8 (2005) 425–439.
- [32] A. S. Jarrah, R. Laubenbacher, A. Veliz-Cuba, The dynamics of conjunctive and disjunctive Boolean network models, Bulletin of Mathematical Biology 72 (2010) 1425–1447.
- [33] L. Mendoza, E. R. Alvarez-Buylla, Dynamics of the genetic regulatory network for *Arabidopsis thaliana* flower morphogenesis, Journal of Theoretical Biology 193 (2) (1998) 307–319.
- [34] L. Mendoza, D. Thieffry, E. Alvarez-Buylla, Genetic control of flower morphogenesis in *Arabidopsis thaliana*: a logical analysis, Bioinformatics 15 (1999) 593–606.
- [35] J. Aracena, M. González, A. Zuñiga, M. A. Mendez, V. Cambiazo, Regulatory network for cell shape changes during drosophila ventral furrow formation, Journal of Theoretical Biology 239 (2006) 49–62.
- [36] C. Georgescu, W. J. R. Longabaugh, D. D. Scripture-Adams, E. S. David-Fung, M. A. Yui, M. A. Zarnegar, H. Bolouri, E. V. Rothenberg, A gene regulatory network armature for T lymphocyte specification, Proceedings of the National Academy of Sciences of the USA 105 (2008) 20100–20105.

- [37] L. Mendoza, F. Pardon, A robust model to describe the differentiation of T-helper cells, Theory in Biosciences 129 (2010) 283–293.
- [38] P. Cull, Linear analysis of switching nets, Biological Cybernetics 8 (1971) 31–39.
- [39] D. A. Huffman, Information theory, Academic Press, 1956, Ch. The synthesis of linear sequential coding networks.
- [40] B. Elspas, The theory of autonomous linear sequential networks, IRE Transactions on Circuit Theory 6 (1959) 45–60.
- [41] E. H. Snoussi, Structure et comportement itératif de certains modèles discrets, Ph.D. thesis, Université Grenoble 1 Joseph Fourier (1980).
- [42] C. Choffrut (Ed.), Automata networks, Vol. 316 of Lecture Notes in Computer Science, Springer, 1988.
- [43] M. Noual, General transition graphs and Boolean automata circuits, Tech. rep., École normale supérieure de Lyon, hal-00452025 (2010).
- [44] M. Noual, Synchronism vs asynchronism in Boolean networks, Tech. rep., École normale supérieure de Lyon, arXiv:1104.4039 (2011).
- [45] M. Noual, S. Sené, Towards a theory of modelling with Boolean automata networks - I. Theorisation and observations, Tech. rep., École normale supérieure de Lyon and Université d'Évry – Val d'Essonne, arXiv:1111.2077 (2011).
- [46] A. Richard, J.-P. Comet, G. Bernot, R. Thomas' modeling of biological regulatory networks: introduction of singular states in the qualitative dynamics, Fundamenta Informaticae 65 (2004) 373–392.
- [47] A. Richard, J.-P. Comet, Necessary conditions for multistationarity in discrete dynamical systems, Discrete Applied Mathematics 155 (2007) 2403–2413.
- [48] J. Demongeot, A. Elena, S. Sené, Robustness in regulatory networks: a multi-disciplinary approach, Acta Biotheoretica 56 (2008) 27–49.
- [49] A. Elena, J. Demongeot, Interaction motifs in regulatory networks and structural robustness, in: Proceedings of CISIS, IEEE, 2008, pp. 682– 686.

- [50] J. Aracena, E. Goles, A. Moreira, L. Salinas, On the robustness of update schedules in Boolean networks, Biosystems 97 (2009) 1–8.
- [51] J. Aracena, É. Fanchon, M. Montalva, M. Noual, Combinatorics on update digraphs in Boolean networks, Discrete Applied Mathematics 159 (2010) 401–409.
- [52] E. Goles, M. Noual, Block-sequential update schedules and Boolean automata circuits, in: Proceedings of Automata 2010, DMTCS, 2010, pp. 41–50.
- [53] E. Goles, M. Noual, Disjunctive networks and update schedules, Advances in Applied Mathematics, 48 646–662.
- [54] F. Robert, Les systèmes dynamiques discrets, Vol. 19 of Mathématiques & Applications, Springer, 1995.
- [55] E. Goles, L. Salinas, Comparison between parallel and serial dynamics of Boolean networks, Theoretical Computer Science 396 (2008) 247– 253.
- [56] E. M. Lederberg, Lysogenicity in *Escherichia coli* strain K-12, Microbial Genetics Bulletin 1 (1950) 5–9.
- [57] H. Eisen, P. Brachet, L. Pereira da Silva, F. Jacob, Regulation of repressor expression in λ , Proceedings of the National Academy of Sciences of the USA 66 (1970) 855–862.
- [58] D. Thieffry, R. Thomas, Dynamical behaviour of biological regulatory networks – II. Immunity control in bacteriophage lambda, Bulletin of Mathematical Biology 57 (1995) 277–297.
- [59] F. Delaplace, H. Klaudel, T. Melliti, S. Sené, Modular organisation of interaction networks based on asymptotic dynamics, Tech. rep., Université d'Évry – Val d'Essonne, arXiv:1111.2313 (2011).
- [60] R. Milo, S. Shen-Orr, S. Itzkovitz, N. Kashtan, D. Chklovskii, U. Alon, Network motifs: simple building blocks of complex networks, Science 298 (2002) 824–827.
- [61] A. W. Rives, T. Galitski, Modular organization of cellular networks, Proceedings of the National Academy of Sciences of the USA 100 (2003) 1128–1133.

- [62] J. Gagneur, R. Krause, T. Bouwmeester, et al., Modular decomposition of protein-protein interaction networks, Genome Biology 5 (2004) R57.
- [63] A. Richard, Negative circuits and sustained oscillations in asynchronous automata networks, Advances in Applied Mathematics 44 (2010) 378– 392.
- [64] R. A. H. Toledo, Linear finite dynamical systems, Communications in Algebra 33 (2005) 2977–2989.