Boolean networks synchronism sensitivity and XOR circulant networks convergence time*

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In this paper are presented first results of a theoretical study on the role of non-monotone interactions in Boolean automata networks. We propose to analyse the contribution of non-monotony to the diversity and complexity in their dynamical behaviours according to two axes. The first one consists in supporting the idea that non-monotony has a peculiar influence on the sensitivity to synchronism of such networks. It leads us to the second axis that presents preliminary results and builds an understanding of the dynamical behaviours, in particular concerning convergence speeds, of specific non-monotone Boolean automata networks called XOR circulant networks.

Keywords. Boolean automata networks, synchronism sensitivity, XOR circulant networks, convergence time.

1 Introduction

Boolean automata networks were first introduced by McCulloch and Pitts in [13] and Kauffman in [11]. These two works and others following these (see [9, 12, 24]) highlighted the importance of embedding biological problematics in a context close to discrete mathematics and theoretical computer science.

In the lines of these studies, we propose in this paper to tackle the question of the role of non-monotony in Boolean automata networks. Our interest in this issue comes from the fact that non-monotony, although widely studied in other contexts [4, 6, 10], is missing from the literature related to Boolean automata networks viewed as models of genetic regulation networks. Indeed, classically, the interaction structure of Boolean models of genetic regulation networks are often represented by *signed* digraphs whose vertices represent genes, and arcs labelled by + (resp. by -) represent activations (resp. inhibitions) of genes on each other. Thus, 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, rather than both. More precisely, it cannot act as an activator under certain circumstances and act as an inhibitor under others. This interpretation of gene regulations

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leads to define monotone Boolean automata networks as studied in [2, 3, 8, 14, 18]. Interesting facts are that, from the general point of view, the global dynamical properties of non-monotone networks have not yet been at the centre of studies in this domain nor has the impact of non-monotone interactions yet been examined *per se*. It therefore seems pertinent to address questions about the role of non-monotony on the dynamical characteristics of Boolean automata networks. To go further, our recent theoretical developments have led us to think that non-monotony may be at the origin of singular behaviours of these networks. This gives additional significance to the issue of non-monotony from both the perspectives of the theory of Boolean automata networks and of the framework of genetic regulation networks. Thus, we present in this paper the grounds of a larger study on non-monotony in networks by developing two lines. The first one consists in understanding the synchronism sensitivity of networks. To do so, we highlight that networks can be synchronism sensitive at different levels and shows that non-monotony is a central structural parameter that helps to classify networks. Then, on the basis of the first line, we present primary results on the dynamical properties (notably in terms of convergence time) of a specific class of non-monotone networks.

In Section 2, we provide definitions and notations of Boolean automata network theory that are used in the paper. Section 3 gives details about a classification of such networks according to their synchronism sensitivity and show that non-monotony is a central parameter in this context. Then, Section 4 presents dynamical properties of XOR circulant networks by exploiting their trajectories and their convergence time. Finally, Section 5 proposes perspectives arising from this work.

2 Definitions and notations

A *Boolean automata network* involves interacting elements. Any of these elements has a state which equals 0 or 1. Then, we speak of inactive and active elements respectively. Moreover, the state of each element can change over time according to the states of other elements and to their influence on it [17, 22]. This section is devoted to the formalisation of the main definitions and notations used in the sequel.

2.1 Network definition

A *Boolean automata network* N of size n is composed of n elements called *automata* which are numbered from 0 to n-1 such that $V = \{0, ..., n-1\}$. Every automaton i has a *state* x_i that takes values in $\{0, 1\}$. The *time space is discrete* and equals \mathbb{N} . The allocation of a value of $\{0, 1\}$ to every automaton of N is called a *configuration* of N. It is represented by a vector $x = (x_0, ..., x_{n-1}) \in \{0, 1\}^n$. We also denote by x(t) (resp. $x_i(t)$) the configuration of N (resp. the state of automaton i) at time step $t \in \mathbb{N}$. The *density* of a configuration x is defined as $d(x) = \frac{1}{n} \cdot |\{x_i \mid (i \in V) \land (x_i = 1)\}|$. Because we are particularly concerned with switches of automata states starting in a given configuration, we introduce the following notations:

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

Notice that $\overline{0}^i$ is the configuration in which $i \in V$ is the only automaton that has state 1 and $\overline{0}^W$ is the configuration in which the automata in W all have state 1 contrary to automata in $V \setminus W$. The interaction structure of N is represented by a digraph G = (V, A), called the *interaction graph* of N that specifies what influences apply to each automaton of N. In G, V equals the set of automata of N and $A \subseteq V \times V$

Figure 1: A Boolean automata network of size 2 with its set of local transition functions and its underlying interaction graph.

is the interaction set. The precise nature of these influences are given by the *local transition functions* $f_i: \{0,1\}^n \to \{0,1\}$ which are associated to each automaton and satisfy:

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

$$\tag{2}$$

In other words, (j,i) is an arc of G if and only if j effectively influences i. This means that in some network configurations (but not necessarily in all of them), the state of j causes a change of states of i. As a consequence, a Boolean automata network is entirely defined by the set of local transition functions of its automata. Figure 1 illustrates a Boolean automata network of size 2 by picturing the set of its local transition functions and its underlying interaction graph.

2.2 Updating modes and transition graphs

The definition of a network does not determine its possible dynamical behaviours. To do so, the way automata are updated over time has to be specified. Here, we introduce the three distinct updating modes that are used in this paper.

The most general standpoint is to consider every possibility. Considering a network *N* as a state transition system, each configuration of *N* is subjected to 2^{n-1} outgoing transitions, one for each non-empty set of automata whose states can be updated. For any subset $W \neq \emptyset \subseteq V$, we define the update function $F_W: \{0,1\}^n \to \{0,1\}^n$ such that:

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

Thus, if we consider the most general updating mode, the global network behaviour is represented by the general transition graph $\mathscr{G}_g = (\{0,1\}^n, T_g)$ where $T_g = \{(x, F_W(x)) \mid x \in \{0,1\}^n, W \neq \emptyset \subseteq V\}$ [15]. In \mathscr{G}_g , an arc is labelled by the list of subsets W of automata that are updated in their corresponding transition $(x, F_W(x))$ such that each F_W applied to x gives the same image (see the left panel of Figure 2).

Transitions $(x, F_i(x))$ that involve the update of one automaton $i \in V$ only are called *asynchronous tran*sitions. Transitions $(x, F_W(x))$, |W| > 1, that involve the update of several are called *synchronous tran*sitions. The sub-graph $\mathcal{G}_a = (\{0, 1\}^n, T_a)$ 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*. Taking \mathcal{G}_a as a reference transition graph allows to define the *asynchronous updating mode* according to which, in each configuration, only *n* transitions 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 [19, 20, 21, 25]. An illustration of an asynchronous transition graph is given in Figure 2 (centre).

The general and the asynchronous transition graphs are very large graphs. In some cases, to draw intuitions, it is interesting to restrict our attention to the transitions resulting from a specific deterministic updating schedule u. This distinct point of view is derived from the work of Robert [22, 23] and has been



Figure 2: (left) General, (centre) asynchronous and (right) parallel transition graphs of the Boolean automata network of Figure 1.

adopted in various studies, see for instance [1, 5, 7]. Section 4 focuses on a specific such deterministic mode, called the *parallel updating mode* π . It consists in updating all automata at once in each network configuration. The underlying 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 $F[\pi]$, *i.e.*, the transition graph $\mathscr{G}_{\pi} = (\{0,1\}^n, T_{\pi})$ where $T_{\pi} = \{(x, F[\pi](x)) \mid x \in \{0,1\}^n\}$ (see the right panel of Figure 2).

2.3 Dynamical behaviours and non-monotony

Consider a Boolean automata network *N* and an updating mode $u \in \{g, a, \pi\}$ among those mentioned above. Let \mathscr{G}_u be the associated transition graph and $x \in \{0, 1\}^n$ be a configuration of *N*. The definitions that follow extend directly and naturally to more general updating modes.

A path in \mathscr{G}_u that starts in x is a *trajectory* of x. In \mathscr{G}_u , strongly connected components that admit no outgoing arcs, called terminal strongly connected components, are called the *attractors* of N. They correspond to the asymptotic behaviours of N. Their sizes equal the number of configurations that they contain. The configurations belonging to attractors of N are called its *recurrent configurations*. An attractor of size 1 is called a *stable configuration*. Other attractors are called *stable oscillations*. In the deterministic context of the parallel update schedule, stable configurations correspond to fixed points of the global transition function $F[\pi]$ and stable oscillations of size p are rather called *limit cycles* of *period* p. They correspond to oriented cycles in \mathscr{G}_{π} . These notions are illustrated in Figure 2. There, stable configurations are represented in light grey and stable oscillations in dark grey. In particular, this figure shows that the network defined in Figure 1 admits a unique stable configuration, that is, configuration 11, whatever the updating mode chosen. This recalls that stable configurations are preserved unlike sustained oscillations (see the limit cycle of period 3 appearing when the network is subjected to the parallel updating mode).

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:

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

or:

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

In other terms, f_i is locally monotone in j if, in the conjunctive (or disjunctive) 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 is a $j \in V$ 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. A network is monotone when all functions f_i , $i \in V$, are monotone. 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). As an example, the network of Figure 1 is partially non-monotone.

3 Synchronism sensitivity and non-monotony

The aim of this section is to focus on the concept of synchronism sensitivity of Boolean automata networks and highlight that non-monotony is a consistent structural parameter that has a significant role in this line.

3.1 Synchronism sensitivity cases

When Boolean automata networks are viewed in the framework of state transition systems by means of the general and asynchronous updating modes, questions about the influence of synchronism on the dynamical behaviours of networks naturally arise. The notion of *synchronism sensitivity* of a network can then be informally described as the fact that its dynamical behaviour changes significantly when synchronism is taken into account in the computation of its evolution. On the basis of the transition graphs \mathcal{G}_a and \mathcal{G}_g (and more precisely on what can change by building \mathcal{G}_g from \mathcal{G}_a), we concentrate on asymptotic dynamical behaviours (and specifically on recurrent configurations rather than attractors). First, we describe the different cases that can possibly occur when synchronous transitions are added to an asynchronous transition graph.

Let N be a Boolean automata network with its associated asynchronous and general transition graphs $\mathscr{G}_a = (\{0,1\}^n, T_a)$ and $\mathscr{G}_g = (\{0,1\}^n, T_g)$ and let $x, y \in \{0,1\}^n$ be two distinct configurations of N. We say that a synchronous transition from $(x, y) \in T_g$ is *sequentialisable* if there exists a sequence of asynchronous transitions from x to y, *i.e.*, if there is a trajectory from x to y in \mathcal{G}_a . It is obvious that if all synchronous transitions of \mathscr{G}_g are sequentialisable then, adding synchronism does not change the asymptotic dynamical behaviour of N and N is then not synchronism sensitive. Let us therefore restrict the study to the case where \mathscr{G}_g contains a non-sequentialisable synchronous transition (x, y). For any $z \in \{0, 1\}^n$, we let \mathscr{A}_z (resp. \mathscr{A}_z^*) be the set of attractors to which z leads or belongs in \mathscr{G}_a (resp. in \mathscr{G}_g). And we denote by $\mathscr{L} = \bigcup_{z \in \{0,1\}^n} \mathscr{A}_z$ (resp. $\mathscr{L}^{\star} = \bigcup_{z \in \{0,1\}^n} \mathscr{A}_z^{\star}$) the set of all attractors in \mathscr{G}_a (resp. in \mathscr{G}_g). With these notations, because of the existence of transition (x, y) in \mathscr{G}_g , any attractor that can be reached by y can also be by x so $\mathscr{A}_{y}^{\star} \subseteq \mathscr{A}_{x}^{\star}$. On the contrary, in \mathscr{G}_{a} , because there are no trajectories from x to y ((x,y) is non-sequentialisable), $\mathscr{A}_y \subsetneq \mathscr{A}_x$ is impossible. Indeed, either (i) y is transient and the only attractors that it can reach are those of $\mathscr{A}_y = \mathscr{A}_x$ that can be reached from x, either (ii) y is transient and it can reach attractors in $\mathscr{A}_y \setminus \mathscr{A}_x \neq \emptyset$ that cannot be reached from x, or (*iii*) y is recurrent and since there are no trajectories from x to y, there also are no trajectories from y to x also is and $\mathscr{A}_x \cap \mathscr{A}_y = \emptyset$. Notice that, in the two latter cases induce $\mathscr{A}_v \not\subseteq \mathscr{A}_x$ and that (i), (ii) and (iii) respectively yield cases 2, 3 and 4 listed below. Thus, when the non-sequentialisable synchronous transition (x, y) is added to \mathcal{G}_a , one of the only four possible cases listed below holds:

- 1. *x* is transient in \mathscr{G}_a . Consequently, the set $\mathscr{L} = \mathscr{L}^*$ of all attractors is unchanged. All configurations $z \in \{0,1\}^n$ that can reach *x* in \mathscr{G}_a , including *x*, remain transient but gain the possibility to reach attractors in $\mathscr{A}_y \setminus \mathscr{A}_z$ (*i.e.*, $\mathscr{A}_y = \mathscr{A}_y^*$ and $\mathscr{A}_x \subseteq \mathscr{A}_z \implies \mathscr{A}_z^* = \mathscr{A}_z \cup \mathscr{A}_y$).
- 2. *x* is recurrent, *y* is transient and $\mathscr{A}_y = \mathscr{A}_x$. Consequently, all $z \in \{0,1\}^n$ on a trajectory from *y* to \mathscr{A}_x , including *y*, become recurrent and are included in \mathscr{A}_x^* , causing \mathscr{A}_x to grow (to become \mathscr{A}_x^*).
- 3. *x* is recurrent, *y* is transient and $\mathscr{A}_y \setminus \mathscr{A}_x \neq \emptyset$. Then *x* becomes transient causing \mathscr{L} to loose attractor $\mathscr{A}_x (\mathscr{A}_x^* = \mathscr{A}_y = \mathscr{A}_y^* \text{ and } \mathscr{L}^* = \mathscr{L} \setminus \mathscr{A}_x)$.
- 4. both x and y are recurrent in \mathscr{G}_a . Attractor \mathscr{A}_x "empties itself" in \mathscr{A}_y ($\forall z \in \mathscr{A}_x, z$ becomes transient and such that $\mathscr{A}_z = \mathscr{A}_x \nsubseteq \mathscr{A}_z^* = \mathscr{A}_y^*$) also causing \mathscr{L} to loose attractor \mathscr{A}_x (to become \mathscr{L}^*).

3.2 Synchronism sensitivity levels

The four cases above suggest between three and four levels of sensitivity (see Definition 1 below) that a Boolean automata network can have to the addition of synchronism (the relative importance of levels 1° and 1° being disputable, they are deliberately not ordered). Cases 1 and 2 respectively yield levels 1° and 1° and 1° and 4 both yield level 2.

Definition 1. Let N be a Boolean automata network. The synchronism sensitivity of N can be of:

- level 0: N is not sensitive at all. All its synchronous transitions either act as shortcuts for asynchronous trajectories or, on the contrary, add local, confluent deviations which increase the number of possible steps in a trajectory without changing its outcome.
- level 1°: N is sensitive in the sense that the addition of synchronism grants additional liberty in the evolutions of some transient configurations that are made to reach a greater number of different attractors.
- level 1[•]: *N* is sensitive in the sense that the addition of synchronism causes some transient configurations to become recurrent and thus some (necessarily unstable) attractors to grow.
- level 2: N is sensitive in the sense that the addition of synchronism destroys attractors.

As said before, because we focus here exclusively on recurrent configurations, the only networks that we have to consider are of levels 1[•] and 2. However, our recent studies have shown that, contrary to level 2, level 1[•] comprises many networks. It is thus not sufficiently discriminant and consequently not significant in our framework. So, let us concentrate on level 2.

3.3 Synchronism sensitive minimal networks

Focusing on synchronism sensitive Boolean automata networks of level 2, our aim is now to show what are the minimal networks (in terms of size) which are sensitive to the addition of synchronism and how they relate to non-monotony. Here, the motivation directly comes from systems and synthetic biology where the discovering of minimal genetic interaction patterns with singular dynamical properties (*i.e.*, singular biological functionalities) seems central to improve our understanding of living organisms.

This leads us to the following proposition.

Proposition 1. *The minimal Boolean automata networks that are synchronism sensitive of level 2 are totally non-monotone.*



Figure 3: (top) Generic description of the four smallest Boolean automata networks that satisfy the conditions of Proposition 1. (bottom) Generic (left) asynchronous and (right) general transition graphs of these networks.

Proof. As explained above, in order to be synchronism sensitive of level 2, a Boolean automata network needs to have at least one non-sequentialisable synchronous transition in its general transition graph \mathscr{G}_g . Let us uncover the structural conditions that must be satisfied by a minimal network N belonging to level 2, with at least one non-sequentialisable synchronous transition. First, N needs to have more than one automaton because, if not, synchronism has no sense. If it has size 2, then, to have a non-sequentialisable synchronous transition, \mathscr{G}_g needs to contain a generic sub-graph (with asynchronous transitions only) of the following form:



where $\bar{x}^{i,j} = \bar{x}^{\{i,j\}} = \bar{x}^{i,j}$ (see Equation 1). This sub-graph is the smallest that is necessary for the general transition graph to contain a non-sequentialisable synchronous transition $(x, \overline{x}^{i,j})$. It is also easy to see that there can be only one non-sequentialisable synchronous transition in the general transition graph \mathcal{G}_{ϱ} of a network of size and level 2. Moreover, to guarantee synchronism sensitivity of level 2, because fixed points are conserved whatever the updating mode, the synchronous transition $(x, \bar{x}^{i,j})$ must go out of a set of configurations belonging to an asynchronous stable oscillation. Now, there is only one way to create an asynchronous stable oscillation that verifies the presence of the asynchronous sub-graph drawn above. It consists in adding transitions (\bar{x}^i, x) and (\bar{x}^j, x) . On this basis, in order to create synchronism sensitivity of level 2, configuration $\bar{x}^{i,j}$ needs to be a fixed point of N. If not, $\bar{x}^{i,j}$ is a predecessor of the limit cycle and adding synchronism will maintain the recurrence of every asynchronous recurrent configuration. Thus, since $\bar{x}^{i,j}$ is a fixed point of N, adding transition $(x, \bar{x}^{i,j})$ makes $\bar{x}^{i,j}$ become the only attractor of N with respect to the general updating mode. Thus, the general transition graph of N must have the form pictured in the bottom right panel of Figure 3 (the bottom left panel illustrates the asynchronous transition graph of such a N to compare). Hence, 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 connector¹. 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 minimal networks satisfying the properties of Proposition 1. They have size 2 and their interaction

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

graphs equal the graph pictured in the top panel of Figure 3. Their two local interaction functions f_0 and f_1 either equal $x \mapsto x_0 \oplus x_1$ or $x \mapsto \neg(x_0 \oplus x_1)$.

Among the four minimal Boolean automata networks described in the proof above that are synchronism sensitive of level 2, those defined by

$$\begin{cases} f_0(x) = x_0 \oplus x_1 \\ f_1(x) = \neg(x_0 \oplus x_1) \end{cases} \text{ and } \begin{cases} f_0(x) = \neg(x_0 \oplus x_1) \\ f_1(x) = x_0 \oplus x_1 \end{cases}$$

are isomorphic. This result relates intimately synchronism sensitivity to non-monotony. Indeed, the smallest patterns that produce synchronism sensitivity strong singularities are non-monotone networks. Moreover, it is easy to see that synchronism sensitivity of level 2 applies to other non-monotone networks. Thus, it would be judicious and interesting to go further and characterise the family of synchronism sensitive non-monotone networks of level 2. Now, in order to develop intuition about the dynamical behaviour of general non-monotone networks, we choose to focus on a specific class of non-monotone networks, namely XOR circulant networks.

4 XOR circulant networks

Let us focus now on the trajectorial and asymptotic dynamical behaviours of XOR circulant networks. These networks define a class of non-monotone Boolean automata networks that is not too large but has all the necessary properties to present complex behaviours.

4.1 Definitions and basic properties

A matrix \mathscr{C} of order *n* whose i^{th} row vector \mathscr{C}_i (*i* < *n*) is the right-cyclic permutation with offset *i* of its first row vector \mathscr{C}_0 so that \mathscr{C} has the following form:

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

is a *circulant matrix*. For any integer $k \ge 2$, a k-XOR *circulant network* of size $n \ge k$ is a network with n automata so that the following four properties are satisfied:

- (1) the adjacency matrix \mathscr{C} of the network interaction graph G = (V,A), called the *interaction matrix*, is a circulant matrix;
- (2) each row \mathscr{C}_i of this matrix contains exactly k non-null coefficients;
- (3) $\mathscr{C}_{0,n-1} = c_{n-1} = 1;$
- (4) the local transition function of any automaton *i* is a XOR function such that $\forall x \in \{0,1\}^n$, $f_i(x) = \bigoplus_{j \in V} \mathscr{C}_{i,j} \cdot x_j = \sum_{j \in V} \mathscr{C}_{i,j} \cdot x_j \mod 2$.

Here, XOR circulant networks are subjected to the *parallel updating mode*, which means that if x = x(t) is the configuration at time step t, then the network configuration at time step t + 1 equals $x(t + 1) = F(x) = \mathscr{C} \cdot x$ (where operations are taken modulo 2). Notice that F is then a linear function [4, 6, 26]



Figure 4: (left) A 2-XOR circulant network of size 4 and (right) a 3-XOR circulant network of size 6.

and that, consequently, a XOR circulant network is entirely defined by its interaction graph G = (V,A) or by its interaction matrix \mathscr{C} . Figure 4 pictures two interaction graphs, the first one (left panel) is a 2-XOR circulant network of size 4, the second is a 3-XOR circulant network of size 6.

A k-XOR circulant network N can be viewed as a *cellular automaton*. Indeed, if N has size n and interaction graph G = (V, A), N can be modelled by the finite one-dimensional cellular automaton of n cells assimilated to the *n* automata of N and that satisfies what follows. The *neighbourhood* \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 similar to the local transition functions of N and is defined as $\gamma((x_{\ell})_{\ell \in \mathscr{N}}) = \bigoplus_{\ell \in \mathscr{N}} x_{\ell}$. We make specific use of this formalisation to exploit tools of 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 $\{0,1\}^n \times \mathbb{N}$ whose line $t \in \mathbb{N}$ represents x(t). The *trace* of cell or automaton i then corresponds to column i of this grid, that is, to the sequence $(x_i(t))_{t \in \mathbb{N}}$. Furthermore, for an arbitrary configuration x and an automaton i, $R_i(x)$ denotes the configuration that satisfies $\forall j \in V$, $R_i(x)_j = x_{2i-j \mod n}$ and is called the *reflection of x* with respect to *i*. We write N to denote the *reflection of N*, *i.e.*, the k-XOR circulant network whose interaction matrix is ${}^{t}\mathscr{C}$. In the sequel, unless it is made explicit, $\mathcal{N}^{-}(i)$ (resp. $\mathcal{N}^{+}(i)$) denotes the *in-neighbourhood* (resp. the *outneighbourhood*) of automaton i and $\widetilde{\mathcal{N}}^{-}(i)$ (resp. $\widetilde{\mathcal{N}}^{+}(i)$) denotes its in-neighbourhood (resp. its outneighbourhood) in \widetilde{N} . Thus, for any two automata $i, j, j \in \mathcal{N}^{-}(i) \iff j \in \widetilde{\mathcal{N}^{+}}(i)$. \widetilde{F} denotes the global transition function of \widetilde{N} if F denotes that of N. Notice that \widetilde{F} represents the reflected global transition function of N. 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, *i.e.*, so that $c_{n-1} = \mathscr{C}_{0,n-1} = 1$. This way, $\{(i, i+1 \mod n) \mid i \in V\} \subseteq A$ defines a Hamiltonian circuit in the structure of N and $\{(i+1 \mod n, i) \mid i \in V\} \subseteq A$ defines a Hamiltonian circuit in the structure of its reflection N.

Let us now list in the proposition below 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 $\binom{n-1}{k-1}$.

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 and it is 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 what follows, 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

Here, 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, let $M_i(t)$ denote the set of automata which have state 1 in configuration $\widetilde{F}^t(\overline{0}^i)$. Then, $\forall x(0) \in \{0,1\}^n, \forall t \in \mathbb{N}, x_i(t) = \bigoplus_{j \in M_i(t)} x_j(0)$.

Proof. We prove Lemma 1 by induction on $t \in \mathbb{N}$. 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 $y(t+1) = \widetilde{F}^{t+1}(y(0)) = \widetilde{F}^t(y(1))$, the induction hypothesis applied 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, because the XOR connector is commutative and associative, we have:

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

Now, remark that $\forall t \in \mathbb{N}$, $\widetilde{F}(\overline{0}^{M_i(t)}) = \overline{0}^{M_i(t+1)}$ by definition. Then, $\forall \ell \in V, \overline{0}_{\ell}^{M_i(t+1)} = 1$ if and only if $|\widetilde{\mathcal{N}}^-(\ell) \cap M_i(t)| \equiv 1 \mod 2$. From this, we derive that $y_i(t+1) = \bigoplus_{j \in M_i(t+1)} y_j(0)$ and then $\forall t \in \mathbb{N}$, $x_i(t) = \bigoplus_{j \in M_i(t)} x_j(0)$.

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 and for any configuration $x \in \{0,1\}^n$, $\widetilde{F}(R_i(x)) = R_i(F(x))$ holds.

Proof. For any automaton *j*, the following holds:

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

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

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

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 and for the initial configuration $x(0) = \overline{0}^i$, it holds that $\forall t \in \mathbb{N}, \widetilde{F}^t(x(0)) = R_i(x(t))$.



Figure 5: Space-time diagrams (a) of a 2-XOR circulant network of size 14 and interaction-step s = 0 (cf. page 48), (b) of its reflected network and (c) of another 2-XOR circulant network of size 27 and interaction-step 4.

Proof. Proposition 3 is proven by induction on *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*. 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.

This result comes from 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 5). Proposition 3 implies that, for any automaton i, the space-time diagram of $(\overline{0}^{i}(t))_{t \in \mathbb{N}}$ is the reflected space-time diagram of $(\overline{0}^{M_{i}(t)})_{t \in \mathbb{N}}$ 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. This is notably due to the fact that configurations of density $\frac{1}{n}$ are unit vectors and because of the underlying superposition principle for linear maps. That leads us to give the following proposition.

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 divides p_* .

Proof. All configurations of density $\frac{1}{n}$ are cyclic permutations of each other. Thus, by Proposition 2.4 their trajectories are isomorphic. They consequently reach their attractor of period p_* at the same time t_* . Now, let x be an arbitrary configuration and i an automaton. By Proposition 3, the space-time diagram of $(\overline{0}^{M_i(t)})_{t\in\mathbb{N}}$ is the reflected space-time diagram of $(\overline{0}^i(t))_{t\in\mathbb{N}}$ with respect to i. Thus, the space-time diagram of $(\overline{0}^{M_i(t)})_{t\in\mathbb{N}}$ reach its attractor at time t_* and its period is p_* . This means that, $\forall i \in N$, the trace of automaton i has period p_* and enters its cyclic behaviour before t_* . As a result, the trajectory of x reaches its attractor before t_* and the period of the latter divides p_* .

4.2.2 2-XOR circulant networks

Now, we focus on 2-XOR circulant networks of arbitrary size *n* and pay attention to the space-time diagrams of configurations of density $\frac{1}{n}$. What is called the *interaction-step* of such a network *N* is the smallest integer $s \neq 1 < n$ such that $\forall i \in V$, $(i, i+s) \in A$. Figure 5 (*a*) and (*b*) illustrates as expected that when s = 0 the space-time diagram is the Sierpinski triangle. For other values of *s*, space-time diagrams are deformed Sierpinski triangles. These observations result in the following lemma (that is used further to analyse 2-XOR circulant networks of size $n = 2^p$, $p \in \mathbb{N}^*$, and interaction step s = 0).

Lemma 3. If N is a 2-XOR circulant network of size n with interaction-step s = 0 then $\forall i \in V, \forall q \in \mathbb{N}, x_i(2^q) = x_{(i-2^q)}(0) \oplus x_i(0)$.

Proof. Lemma 3 is proven by induction on q. Let $i \in V$ be an arbitrary automaton and let q equal 1 initially. Clearly, the following holds:

$$x_i(2) = x_{(i-1)}(1) \oplus x_i(1) = x_{(i-2)}(0) \oplus x_{(i-1)}(0) \oplus x_{(i-1)}(0) \oplus x_i(0) = x_{(i-2)}(0) \oplus x_i(0).$$

Thus, the basis of the induction holds too. Now, consider that, for $q \in \mathbb{N}$, $x_i(2^q) = x_{(i-2^q)}(0) \oplus x_i(0)$ is true. In the sequel, we pay particular attention to states

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

Then, by induction hypothesis, for q + 1, we have $d = a \oplus b$, $e = b \oplus c$ and $f = d \oplus e$, from which we derive that $f = d \oplus e = (a \oplus b) \oplus (b \oplus c) = a \oplus c$. As a result, we can write:

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

and obtain the expected result.

4.2.3 2-XOR circulant networks of sizes powers of 2

In this paragraph, we restrict the study to 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*. *x* can be viewed 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 $x'' = (x_{\frac{n}{2}}, \ldots, x_{n-1})$. *x'* and *x''* are called the *semi-configurations* of *x*. Let us define the *repetition degree* $\delta_r(x)$ of *x* as:

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

x is said to be a *repeated configuration* when x = (x', x'). Moreover, remark that the time complexity for computing the repetition degree is $\mathcal{O}(n)$. Let us now present results about such networks convergence times.

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 $\log_2(n) - 1$, namely, $(0, 1, \dots, 0, 1)$, 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 $t \in \mathscr{T}$ and let x(t) be either $(0,1,\ldots,0,1)$ or $(1,0,\ldots,1,0)$. If *s* is even, then, by hypothesis on x(t), $\forall i \in V$, $x_{(i+s)}(t+1) = x_i(t) \oplus x_{(i+s-1)}(t) = 1$. Otherwise, if *s* is odd, then, $\forall i \in V$, $x_{(i+s)}(t+1) = x_i(t) \oplus x_{(i+s-1)}(t) = 0$. Now, considering with this Propositions 2.2 and 2.3, we get the expected result.

Let us now focus on the particular case of 2-XOR circulant networks of sizes $n = 2^p$, $p \in \mathbb{N}^*$, and interaction-steps s = 0.

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

Proof. Since $n = 2^p$, by Lemma 3, $\forall i \in V$, $x_i(n) = x_i(0) \oplus x_{i+n}(0) = x_i(0) \oplus x_i(0) = 0$. Then, any configuration *x* converges to the stable configuration $(0, \dots, 0)$ in no more than *n* time steps.

Questioning about the configurations whose convergence time is maximal leads us to Lemma 4 and Theorem 2.

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. Let *x* be an arbitrary repeated configuration of *N*. By induction on *t*, we show that $\forall t \in \mathbb{N}$, x(t) = (x'(t), x'(t)). Let G' = (V', A') be the interaction graph of *N'*. By hypothesis, the lemma is true for t = 0. Now, consider that x(t) = (x'(t), x'(t)) for $t \in \mathbb{N}$ (x(t) is a repeated configuration) and that $\forall i \in V$, $x_i(t+1) = x_{(i-1)}(t) \oplus x_i(t)$. Hence we have, for all $i \in V$:

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

Consequently, x(t+1) is also repeated and verifies, for all $i \in V'$:

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

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

Theorem 2. 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] converges in n time steps exactly.

Proof. We proceed 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, the basis of the induction holds. Consider the following induction hypothesis: for p = q, any configuration x such that $2^q \cdot d(x) \equiv 1$ [2] converges in 2^q time steps. Suppose now 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]. After 2^q time steps:

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

• x' has an odd number of 1s. By the property above together with Lemma 3, since $\forall i \in \{0, \dots 2^q - 1\}, x'_i(2^q) = x_i(2^q) = x_i(0) + x_{(i+2^q)}(0)$, 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 $x'(2^q)$. Furthermore, by the induction hypothesis, x' converges in exactly 2^q time steps. Hence, x converges in exactly $n = 2^{q+1}$ time steps.

5 Conclusion and Perspectives

In this paper, we have highlighted that non-monotony could be at the origin of dynamical singularities of Boolean models of genetic regulation networks, with respect to their sensitivity against synchronism. This is an interesting property because biological experimentations currently give no tangible results about the way that genes express over time. Moreover, on the basis of this result, we have developed a study on the XOR circulant networks class and have shown some notable results about their convergence times in particular.

This work opens many research directions that could help develop the knowledge on the influence of non-monotony in automata networks and, *a fortiori*, in real genetic networks. One of these perspectives relies on the first part of this paper dealing with synchronism sensitivity. It would consist in understanding how do monotone and non-monotone Boolean automata networks relate. In [16], preliminary results are derived on synchronism sensitivity of monotone networks that emphasise necessary structural conditions (namely, the presence of specific circuits in the interaction graphs) and examples of synchronism sensitive monotone networks are given. What is interesting is that these examples involve linear *monotone codings* of non-monotony. This naturally raises the question of whether non-monotony accounts for the synchronism sensitivity in arbitrary monotone and non-monotone networks. In addition, further analyses on the behaviours of XOR circulant networks are planned. We would like to obtain generalisations of the results presented above by following two directions: relaxing structural constraints step by step and viewing these networks as state transition systems rather than discrete dynamical systems subjected to the parallel updating mode.

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