Phase transitions in stochastic non-linear threshold Boolean automata networks on $\mathbb{Z}^2$: the boundary impact

Jacques Demongeot, Sylvain Sené

Phase transitions in stochastic non-linear threshold Boolean automata networks on $\mathbb{Z}^2$: the boundary impact

Jacques Demongeot[1], Sylvain Sené[2]

[1] Université Grenoble – Alpes, CNRS, AGIM FRE3405, La Tronche, France
[2] Aix-Marseille Univ., Toulon Univ., CNRS, LIS UMR7020, Marseille, France

Abstract

This paper addresses the question of the impact of the boundary on the dynamical behaviour of finite Boolean automata networks on $\mathbb{Z}^2$. The evolution over discrete time of such networks is governed by a specific stochastic threshold non-linear transition rule derived from the classical rule of formal neural networks. More precisely, the networks considered in this paper are finite but the study is done for arbitrarily large sizes. Moreover, the boundary impact is viewed as a classical definition of a phase transition in probability theory, characterising in our context the fact that a network admits distinct asymptotic behaviours when different boundary instances are assumed. The main contribution of this paper is the highlight of a formula for a necessary condition for boundary sensitivity, whose sufficiency and necessity are entirely proven with natural constraints on interaction potentials.

Keywords: Boolean automata networks, non-linearity, stochastic processes, phase transitions, boundary sensitivity.

1 Introduction

Understanding the influence of the frontiers (or boundaries, or environment) of systems composed of interacting entities is a problem born in the 1920's. In physics, after the seminal parper of Ising in 1925 dealing with phase transitions in ferromagnetic systems [26] and the first theoretical proof of their existence by Onsager in 1944 [34], the most important works on this subject are certainly those that focused at the end of the 1960's on lattice gas models. Amongst these works, those of Dobrushin [17, 18] and Ruelle [38, 39] are obviously the most known in the sense that they presented the first results proving that the Ising model embedded into a square lattice admits a phase transition depending on the nature of its boundary conditions. Even if these works were dived in physics, they opened many questions in other disciplines. Indeed, issues underlying the role of boundaries on systems is all the more pertinent in frameworks at the frontier of theoretical computer science and biology. For instance, boundary conditions may allow to represent the post-transcriptional actions of non-coding RNAs in the genetic context [27], external electric fields in the neural context [3], and also hormone flows control in both of these [11].

Since decades, researches in discrete mathematics and fundamental computer science have put the emphasis on the modelling abilities of automata networks concerning interaction networks. In particular, since their introduction in the works of McCulloch and Pitts [31] and Kauffman [29, 28], Boolean automata networks (BANs for short) have been at the centre of numerous studies in the field of biological networks modelling, like neural networks [20, 24, 25, 21, 9, 8], genetic regulation networks [30, 43, 44, 41, 32, 4, 36] and more recently social networks [16, 12]. This can be easily explained by their very high level of abstraction that makes them ideal objects to capture formally the essence of interactions and to focus on qualitative aspects of their dynamics (*e.g.*, the information transmissions).

In this paper, our attention has focused on a fundamental analysis of the asymptotic dynamical behaviours of a particular class of BANs on $\mathbb{Z}^2$ subjected to the influence of distinct boundary instances. Previous works on *linear stochastic threshold* BAN*s* (LSBANs for short) showed that the sensitivity of such BANs against their boundary is quite similar to that of the Ising model [13, 14]. In the same lines and on the basis of preliminary results [15], the main contribution of this paper is an explicit formula of a necessary condition according to which *non-linear stochastic threshold* BAN*s* (NSBANs for short) are effectively subjected to the impact of changes of their boundary instances. Our interest in non-linearity comes from the fact that non-linearity is an original way to model entity coalitions. For instance, about biological regulation networks, it gives a way to represent protein complexes [32, 2, 7] inside the local transition functions, which prevents from transforming the structural features of networks by adding vertices and edges to their underlying interaction graphs. Thus, non-linearity constitutes a means to explicit cooperative or competitive coalitions without increasing problem sizes (*i.e.*, the sizes of their inputs).

First, in Section 2, we give the main definitions and notations used throughout the paper, by basing ourselves on the classical model of LSBANs. Then, Section 3 presents the complete description of non-linear stochastic BANs considered in this paper. After that, in Section 4, we develop the intermediary results that lead to the explicit formula characterising the condition that is necessary for NSBANs to be structurally sensitive to their boundary instances. Then, a discussion highlighting perspectives of this work concludes the paper.

2 Definitions and notations

2.1 Classical stochastic threshold BANs

Before we define formally NSBANs, for the sake of clarity and in order not to burden the reading, let us present every useful concept in the context of LSBANs.

The *geometric structure* of a LSBAN N of size n on $\mathbb{Z}^2$ is given by a connected undirected graph $G = (V, E)$, where $V = \{0, \dots, n-1\} \subseteq \mathbb{Z}^2$ is the set of automata, and $E \subseteq \{\{i, j\} \mid i, j \in V\}$ is the set of edges that connect automata of N so that $\forall i, j \in V,\ \{i, j\} \in E \iff d_{L_1}(i, j) \leq 1$, where d_{L_1} is the L_1 distance. Informally, each automaton of V is connected to itself and its nearest automata, which means that N is defined according to the von Neumann neighbourhood from the cellular automata standpoint [45]. The *complete structure* of N is obtained by associating with every edge $\{i, j\} \in E$ a label $w_{\{i,j\}} \in \mathbb{R}_{\neq 0}$ (the non-zero real numbers) that is called the *interaction weight* between i and j and by relating to G a vector θ of dimension n taking values in $\mathbb{R}^n$. In the sequel, we make particular use of the notion of neighbourhood and distinguish the *neighbourhood* $\mathcal{N}_i$ of automaton i defined as $\mathcal{N}_i = \{j \mid \{i, j\} \in E\}$ from the *strict neighbourhood* $\mathcal{N}_i^*$ of automaton i defined as $\mathcal{N}_i^* = \{j \neq i \mid \{i, j\} \in E\}$. Furthermore, each automaton evolves according to a common transition function. This is ensured by the fact that, in the sequel, the complete structure of every N considered satisfies isotropy, translation invariance, and $\forall i, j \in V,\ \theta_i = \theta_j$. Notice that *(i)* N is *isotropic* if and only if $\forall i, j, j' \in V,\ j, j' \in \mathcal{N}_i^*,\ w_{\{i,j\}} = w_{\{i,j'\}}$, and that *(ii)* N is *translation invariant* if and only if $\forall i, i' \in V,\ s = i' - i,\ \forall j \in \mathcal{N}_i,\ w_{\{i,j\}} = w_{\{i',j+s\}}$.

Since we focus on BANs, the state x_i of each automaton i of N can take values in $\{0, 1\}$. Because of the discrete nature of time, abusing language, the state of automaton i at time step $t \in \mathbb{N}$ is denoted by $x_i(t)$. From this, we derive that the configuration space of N is $\{0, 1\}^n$ and denote by vector

$x(t)$ of dimension n (where $x(t) = (x_i(t))_{i \in V} \in \{0,1\}^n$) the *configuration* of N obtained from the initial configuration $x = x(0)$ after t time steps. Now, let us introduce the classical definition of the transition function of a LSBAN that is a generalisation of the Boltzmann machine [1, 23] to the framework of threshold BANs. It defines $P(x_i(t+1) = 1 \mid x(t))$ that is the conditional probability for automaton i to be in state 1 at time step $t+1$, knowing the states of its neighbours at time t, such that:

$$\forall i \in V,\, \forall t \in \mathbb{N},\; P(x_i(t+1) = 1 \mid x(t)) = \frac{e^{(\sum_{j \in \mathcal{N}_i} w_{\{i,j\}} \cdot x_j(t) - \theta_i)/T}}{1 + e^{(\sum_{j \in \mathcal{N}_i} w_{\{i,j\}} \cdot x_j(t) - \theta_i)/T}}, \quad (1)$$

where θ_i is the *threshold* of automaton i and $T \in \mathbb{R}^+$ is a temperature parameter and allows to make the network studied "more or less probabilistic". Indeed, when T tends to 0, the transition function above is equivalent to the classical deterministic one [31, 19], except for the value 0 of the exponent of the exponential, for which the choice is not 0, but 1 or 0 with probability $\frac{1}{2}$; when it tends to $+\infty$, the probability for the state of any automaton to be equal to 1 is $\frac{1}{2}$.

2.2 Centre, boundary and simplifications

Classically, in graph theory [22, 6], the notions of boundary and centre are defined for directed graphs as follows, considering a directed graph $G = (V, E)$. The *boundary* of G is the set of its sources, a *source* of a directed graph $G = (V, E)$ being a vertex $i \in V$ whose number of inward edges equals 0. Now, let $G = (V, E)$ be a connected directed graph, let $i, j \in V$ and let us define a vertex $i \in V$ as a *sink* if the number of its outward edges equals 0. The *graph distance* $d(i, j)$ from i to j equals the length of the shortest path from i to j if this path exists and $+\infty$ otherwise. The *eccentricity* $\varepsilon(i)$ of vertex i is defined as:

$$\varepsilon(i) = \begin{cases} \mathrm{Max}_{j \in V \setminus \{i\}}(d(i,j) < +\infty) & \text{if } i \text{ is not a sink,} \\ +\infty & \text{otherwise.} \end{cases}$$

From this, the *centre* of G is the set of its vertices of minimal eccentricity. Let us now explain how to adapt these definitions in our context, considering an arbitrary LSBAN N with its associated interaction graph $G = (V, E)$.

First of all, remark that the definition of the *centre* adapts easily to N. Indeed, it suffices to use punctually the matching directed version $N_\triangleright$ of N and its associated interaction graph $G_\triangleright = (V, E_\triangleright)$ whose edge set $E_\triangleright \subseteq V \times V$

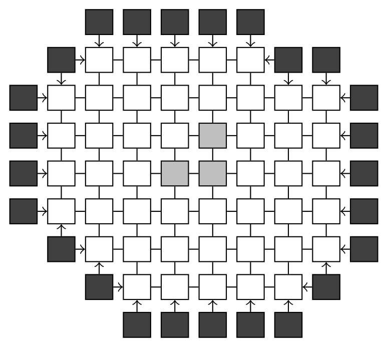

Figure 1: Structure of a system $\mathcal{S}$ in $\mathbb{Z}^2$ built from a BAN N whose automata are represented in white and light grey (central cells) to which have been added boundary automata (in dark grey).

is simply obtained by decoupling every edge of E into two edges so that: $\{i, j\} \in E \implies (i, j), (j, i) \in E_{\triangleright}$. Now, since G is undirected and has consequently no source vertices, N has no boundary in the sense of the definition above. So, to define the boundary of N, here also, we use $N_{\triangleright}$ and $G_{\triangleright}$. Let $V^c = \mathbb{Z}^2 \setminus V$ be the set of vertices that complements V to recover $\mathbb{Z}^2$. The boundary V^{ext} of N is then defined by $V^{\text{ext}} = \{i \in V^c \mid \exists j \in V,\ d_{L_1}(i, j) = 1\}$. The states of elements of V^{ext} remain fixed. From this, we derive that the interaction graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ of the *system* $\mathcal{S}$ that recovers N and V^{ext} is such that $\mathcal{V} = V \cup V^{\text{ext}}$ and $\mathcal{E} = E \cup \{(i, j) \mid i \in V^{\text{ext}}, j \in V,\ d_{L_1}(i, j) = 1\}$. Furthermore, we enforce $\mathcal{S}$ to maintain the isotropy and translation invariance properties of N. That means that $\forall i, j, k \in \mathcal{V}$, $i, j \in V, k \in V^{\text{ext}}$, $d_{L_1}(i, j) = d_{L_1}(i, k) = 1,\ w_{(i,k)} = w_{\{i,j\}}$, where $w_{(i,k)}$ is the interaction weight that k has on i. Thus, by extending the definitions of neighbourhood and strict neighbourhood to $\mathcal{E}$ rather than E only, such an automaton k of $\mathcal{S}$ is a source of $\mathcal{G}$ and is such that $k \in \mathcal{N}_i$ whereas $i \notin \mathcal{N}_k$. Finally, in informal terms, $\mathcal{S}$ is a BAN that is built from N by adding to it peripheral automata that act on N and whose states remain fixed. An illustration of such a system $\mathcal{S}$ is pictured in Figure 1.

For the sake of simplicity in the following analysis and without loss of generality, for any automaton i of N, its threshold θ_i is made null ($\forall i \in V,\ \theta_i = 0$) and its role is played by the self-interaction weight $w_{\{i,i\}}$. Thus, from now on, $w_{\{i,i\}}$ always participates to the computation of the transition function of automaton i, whatever the state of the latter is. From this, we derive a new version of Equation 1 accounting for the notion of boundary:

$$\forall i \in V,\ P(x_i(t+1) = 1 \mid x(t)) = \frac{e^{(w_{\{i,i\}} + \sum_{j \in \mathcal{N}_i^*} w_{\{i,j\}} \cdot x_j(t))/T}}{1 + e^{(w_{\{i,i\}} + \sum_{j \in \mathcal{N}_i^*} w_{\{i,j\}} \cdot x_j(t))/T}}. \tag{2}$$

Before we introduce some notions dealing with probability theory, let us add that this study is restricted to attractive stochastic BANs, *i.e.* BANs that satisfy the following property: $\forall i, j \in V$, $j \in \mathcal{N}_i^*,\ w_{\{i,j\}} > 0$ so that for every $i \in V$, the probability for i to be in state 1 at time $t+1$ knowing the global configuration of the BAN at time t increases proportionately to the number of its neighbours being in state 1.

2.3 Markov chains, invariant measures and phase transitions

From Equation 2, obviously, the dynamical behaviour of an arbitrary LSBAN N of size n (resp. of its associated system $\mathcal{S}$) is a finite *stationary Markov chain* whose random variables are the possible configurations of N (resp. of $\mathcal{S}$) such that:

$$\forall t \in \mathbb{N}^*,\ P(x(t+1) \mid x(t)) \ = \ P(x(t) \mid x(t-1)).$$

Let C be the stationary Markov chain representing the dynamical behaviour of N (*remember that the boundary is not a part of N, since $V^{ext} \not\subseteq V$ by definition*). The *Markovian matrix* p underlying C is the matrix of order 2^n such that:

$$\forall i, j \in \{0,1\}^n,\ \mathsf{p}_{i,j} \ = \ P(x(t+1) = j \mid x(t) = i).$$

Let us now define the notion of invariant measure (or stationary probability distribution). An *invariant measure* of C is a vector μ whose entries are non-negative and sum to 1 that satisfies:

$$\mu_j = \sum_{i \in \{0,1\}^n} \mu_i \cdot \mathsf{p}_{i,j}.$$

In other words, μ is a normalised left eigenvector of the Markovian matrix associated with the eigenvalue 1. A notable fact is that such a μ defines an attractor of C (and consequently of N). Furthermore, by Equation 2, it is obvious that Markovian matrices of LSBANs contain only positive coefficients. As a consequence, the Perron-Frobenius theorem applies and ensures the uniqueness of the invariant measure of N. Now, consider the system $\mathcal{S}$. More precisely, let us consider an *instance* $\mathcal{S}^\circ$ of $\mathcal{S}$ such that the state of each automaton of V^{ext} has been fixed to a value in $\{0, 1\}$ and denote by μ° the invariant measure of N when covered by $\mathcal{S}^\circ$. Consider also another distinct instance $\mathcal{S}^\bullet$ of $\mathcal{S}$ and $\mu^\bullet$. Although the invariant measure of N is unique, $\mu^\circ = \mu^\bullet$ does not hold a priori. As Dobrushin did in [17, 18], we say that a BAN N is *boundary sensitive* if and only if $\mu^\circ \neq \mu^\bullet$. It admits a *phase transition*, if this difference still holds for the limits of these invariance measures when the number of vertices n of N tends to infinity. The existence of a phase transition that corresponds to the persistence of the boundary sensitivity when the size of N tends to infinity can be called *asymptotic boundary sensitivity*.

In what follows, we propose a method to prove a structural parametric condition, based on the asymptote of BANs, that is necessary for boundary sensitiveness. Such a condition defines then a domain of phase transitions. *Notice that the word "asymptote" has to be considered here both on the sizes and the dynamical behaviours.*

2.4 Past results on LSBANs

In [13, 14, 40], we obtained several results on LSBANs in this framework. The major ones, of analytical nature, are described in the three following theorems (the first one deals with the notions of updating modes; for more details, see [40, 37]).

Theorem 1. *Let N be a* LSBAN *and let $W \subseteq V$ a subset of automata be* sparse *if and only if $\forall i, j \in E, i \neq j,\ w_{i,j} = 0$. The emergence of a phase transition from its asymptotic behaviour whatever its size occurs under the same conditions when N evolves according to the parallel updating mode, any of the sequential updating modes and every block-sequential updating mode equivalent to a block-parallel updating mode built recursively from successive subdivisions of N in sparse blocks.*

Theorem 2. *One-dimensional* LSBAN*s do not admit any phase transition in view of their boundaries.*

Theorem 3. *Let N be an arbitrary attractive* LSBAN *on $\mathbb{Z}^2$. If N admits a phase transition in view of its boundary, then N is defined such that $u_{0,i} + 2u_{1,i,j} = 0$, where, $\forall i, j \in V,\ u_{0,i} = \frac{w_{\{i,i\}}}{T}$ and $u_{1,i,j} = \frac{w_{\{i,j\}}}{T}$.*

Theorem 3 gives a necessary condition for the emergence of a phase transition. In order to obtain the characterisation (without proving it however) of the domain of phase transition, we performed an empirical study based on

Monte-Carlo simulations. The conclusions emphasised that the domain is located on a semi-straightline of equation $u_{0,i} + 2u_{1,i,j} = 0$. One of the most interesting points here is that this result is analogous to that found by Ruelle on the ferromagnetic Ising model [39]. Other studies were also led on repulsive LSBANs (*i.e.*, with negative $w_{i,j}$'s). They emphasised that the domain of phase transitions is then located in a large neighbourhood of the semi-straightline $u_{0,i} + 2u_{1,i,j} = 0$, as it has been shown for the anti-ferromagnetic Ising model by Dobrushin [18].

3 Non-linear stochastic BANS

Now that every important notion for the study has been defined and explained, we give precisions about NSBANs. First of all, notice that all the previous definitions extend simply and apply naturally to NSBANs.

3.1 Interaction potentials

Consider an arbitrary two-dimensional LSBAN and Equation 2. For any automaton $i \in V$, we give an important role to two particular parameters, namely the *interaction potentials* $u_{0,i}$ and $u_{1,i,j}$ (cf. definitions above) which provide respectively images of the self-interaction weights and of the strict neighbours interaction weights with respect to the temperature parameter T. The NSBANs we are interested in are such that the evolution of their automata over time does not only account for these two parameters anymore but for three parameters, $u_{0,i}$, $u_{1,i,j}$ and η. Function η (see below) provides the images of *non-linear collective interaction potentials* that neighbour automata can activate when several are in state 1 simultaneously. These collective interaction potentials can thus take different forms according to the configuration in the neighbourhood of automaton i. Notice that nonlinearity has already been addressed on the Ising model considering only triplet potentials [47, 46, 35]. Now, let us define and list below the possible interaction potentials which are taken into account. To do so, let us consider an automaton i of a NSBAN N with its interaction graph $G = (V, E)$ and its underlying covering system $\mathcal{S}$:

- the unique *singleton potential* of i is defined as $u_{0,i} = w_{\{i,i\}}/T$;
- the four possible *couple potentials* of i are defined as $\forall j \in \mathcal{N}_i^*,\ u_{1,i,j} = w_{\{i,j\}}/T$;

– the ten *triplet potentials* of i are defined as $\forall j, \ell \in \mathcal{N}_i,\ j \neq \ell,\ u_{2,i,\langle j,\ell\rangle} = w_{\{i,\langle j,\ell\rangle\}}/T$ (at least two distinct neighbours of i are in state 1);

– the ten *quadruplet potentials* of i are defined as $\forall j, \ell, m \in \mathcal{N}_i,\ j \neq \ell \neq m,\ u_{3,i,\langle j,\ell,m\rangle} = w_{\{i,\langle j,\ell,m\rangle\}}/T$ (at least three distinct neighbours of i are in state 1);

– the five *quintuplet potentials* of i are defined as $\forall j, \ell, m, p \in \mathcal{N}_i,\ j \neq \ell \neq m \neq p,\ u_{4,i,\langle j,\ell,m,p\rangle} = w_{\{i,\langle j,\ell,m,p\rangle\}}/T$ (at least four distinct neighbours of i are in state 1);

– the unique *sextuplet potential* is defined as $\forall i, j, \ell, m, p \in \mathcal{N}_i,\ i \neq j \neq \ell \neq m \neq p,\ u_{5,i,\langle i,j,\ell,m,p\rangle} = w_{\{i,\langle i,j,\ell,m,p\rangle\}}/T$ (every neighbour of i is in state 1).

Since BANs considered are isotropic and translation invariant, let us right now simplify notations and denote the singleton up to sextuplet interaction potentials respectively by u_0, u_1, u_2, u_3, u_4 and u_5. For the sake of clarity and in order to give some insights about these interaction potentials, notice that, for instance, a triplet potential u_2 is the interaction weight normalised by T that automaton i receives from the set of neighbour automata j and ℓ. In other words, it represents the interaction potential that the *group* composed of j and ℓ together (viewed as a new kind of interacting entity) has on i. Remark also that interaction potentials are "cumulative" in the sense that an automaton that is subjected to a triplet potential is also subjected to one or two couple potentials (depending on i belongs or not to the group acting on itself) and its singleton potential (which always takes part in the computation of its new state). Figure 2 illustrates these different interaction potentials and the neighbourhood configurations that make them possible.

3.2 NSBANs definition

From the definition of interaction potentials above, we derive directly that of NSBANs given in Definition 1 below.

Definition 1. *Let $G = (V, E)$ a digraph whose vertices are automata in $\mathbb{Z}^2$. A two-dimensional* NSBAN *N of size n and order k, $2 \leq k \leq 6$, associated with G is a* BAN *whose local transition functions are stochastic and such that:*

$$\forall i \in V,\ P(x_i(t+1) = 1 \mid x(t)) \ = \ h \circ \exp \circ\, p_i(x(t)), \tag{3}$$

where $h(y) = \frac{y}{1+y}$, and $p_i(x(t)) = u_0 + \sum_{j \in \mathcal{N}_i^*} u_1 \cdot x_j(t) + \eta_i^k(x(t))$ is the global interaction potential received by i at time t, and where $\eta_i^k(x(t))$ is called the

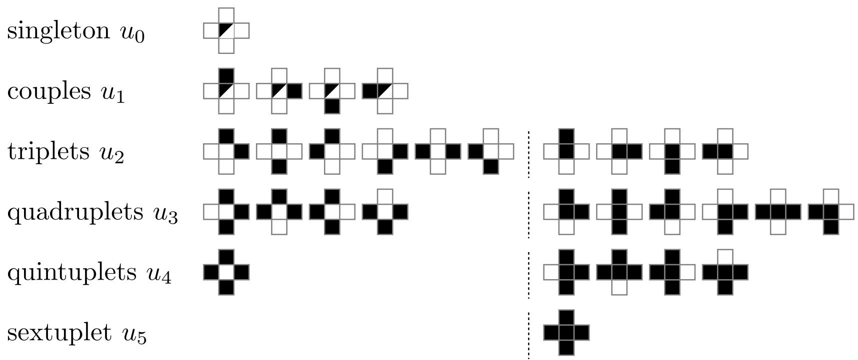

Figure 2: Relations between all the different possible neighbourhood configurations possibles of an arbitrary automaton $i \in V$ of a NSBAN on $\mathbb{Z}^2$ and the interaction potentials they induce. The automata in black (resp. white) represent active automata (resp. inactive automata). In the two first lines related to singleton and couple potentials, automaton i is half-black half-white to make explicit the fact that the singleton potential is taken into account at each time step of the evolution and that the taking into account of couple potentials in the computation of the new state of i at time $t+1$ does not depend on its state at time t but only depends on the states of its strict neighbours at time t (cf. paragraph before Equation 2 at page 5). Furthermore, in the four last lines, we distinguish configurations by putting on the left (resp. on the right) those in which the central automaton is inactive (resp. active).

non-linear term *of N and accounts for collective interaction potentials such that:*

$$\eta_i^k(x(t)) = \begin{cases} 0 & \textit{if } k = 2, \\ \sum_{\substack{j_1, j_2 \in \mathcal{N}_i \\ j_1 \neq j_2}} u_2 \cdot x_{j_1}(t) \cdot x_{j_2}(t) & \textit{if } k = 3, \\ \sum_{\substack{j_1, \ldots, j_{k-1} \in \mathcal{N}_i \\ j_1 \neq \cdots \neq j_{k-1}}} u_2 \cdot x_{j_1}(t) \cdot x_{j_2}(t) + \ldots + & \\ \qquad\qquad u_{k-1} \cdot x_{j_1}(t) \cdot \ldots \cdot x_{j_{k-1}}(t) & \textit{otherwise.} \end{cases}$$

It follows that particular NSBANs of order $k = 2$ are actually LSBANs whereas those of order $k \geq 3$ are effectively non-linear because of their non-null non-linear term and are consequently generalised Boltzmann machines extended to account several kinds of non-linear interaction potentials. From now on, we only focus on NSBANS of order $3 \leq k \leq 6$.

3.3 Transfer matrix

Let $N^\star$ be a NSBAN in $\mathbb{Z}^2$ of size n and order $3 \leq k \leq 6$. We denote its underlying interaction graph by $G^\star = (V^\star, E^\star)$ and its associated Markov chain (whose related Markovian matrix is $\mathsf{p}^\star$) by $\mathsf{C}^\star$. In order to ease the analysis of Section 4, let us give a new notation for configurations based on cylinders of set theory. In the sequel, a configuration $x \in \{0,1\}^n$ is denoted by the cylinder $[A, B] \in \{0,1\}^n$ where $A = \{i \in V^\star \mid x_i = 1\}$ and $B = \{i \in V^\star \mid x_i = 0\}$.

Now, consider the invariant measure μ of $\mathsf{C}^\star$. By definition, μ satisfies the following projective and conditional relations. Projective equations are defined as:

$$\forall [A,B] \in \{0,1\}^n,\ \forall i \in A,\quad \mu([A,B]) + \mu([A \setminus \{i\}, B \cup \{i\}]) = \mu([A \setminus \{i\}, B]),$$

where $\mu([A,B])$ stands for the stationary probability to observe configuration $[A, B]$. *Conditional equations* are defined as:

$$\forall i \in V^\star,\ \mu([\{i\}, \emptyset]) = \sum_{A,B} \Phi_i(A,B) \cdot \mu([A,B]),$$

where $\mu([\{i\}, \emptyset])$ is the stationary probability for automaton i to be in state 1 and $\Phi_i(A, B)$ is the conditional probability given in Equation 3 for automaton i to be in state 1 at time step $t + 1$ knowing configuration $[A, B]$ at time t such that:

$$\mu(x_i(t+1) = 1 \mid [A,B]) \ = \ \Phi_i(A,B) \ = \ h \circ exp \circ p_i([A,B]) \ = \ \frac{e^{u_0 + \sum_{j \in \mathcal{N}_i^* \cap A} u_1 \cdot x_j(t) + \eta_i^k([A,B])}}{1 + e^{u_0 + \sum_{j \in \mathcal{N}_i^* \cap A} u_1 \cdot x_j(t) + \eta_i^k([A,B])}}.$$

From now on, we abuse the notation of η by considering that $\eta_i^k([A,B]) = \eta_i^k(A)$ for not weighting down the writing of equations. Furthermore, by hypothesis of the translation invariance property, $N^\star$ owns a spatial Markovian character that allows to study its dynamical behaviour by analysing only that of the sub-NSBAN N of size 5 whose interaction graph $G = (V, E)$ is the sub-graph of $G^\star$ restricted to the vertices in the neighbourhood $\mathcal{N}_o$ of one arbitrary central automaton o of $N^\star$[1]. Consider that the four automata

[1] Notice that the choice of a central node is not mandatory in this theoretical framework

of the strict neighbourhood of o are distinguished lexicographically so that $\mathcal{N}_o^* = \{1,2,3,4\}$. Notice that, because the following analysis needs it, the concept of cylinder $[A,B]$ is restricted to automata of $\mathcal{N}_o^*$, *i.e.*, $A, B \subseteq \mathcal{N}_o^*$, so that the non-linear term becomes:

$$\eta_i^k(A) = \begin{cases} \sum_{\substack{j_1,j_2 \in \mathcal{N}_i \cap (A \cup \{o\}) \\ j_1 \neq j_2}} u_2 \cdot x_{j_1}(t) \cdot x_{j_2}(t) & \text{if } k=3, \\ \sum_{\substack{j_1,\ldots,j_{k-1} \in \mathcal{N}_i \cap (A \cup \{o\}) \\ j_1 \neq \ldots \neq j_{k-1}}} u_2 \cdot x_{j_1}(t) \cdot x_{j_2}(t) + \ldots + & \\ \qquad\qquad u_{k-1} \cdot x_{j_1}(t) \cdot \ldots \cdot x_{j_{k-1}}(t) & \text{otherwise.} \end{cases}$$

Let us now introduce the concept of positive *transfer matrix*, whose definite character and phase transition existence are related.

Definition 2. *Let $N^\star$ be a* NSBAN *of size n and order k on $\mathbb{Z}^2$. Let N be the restriction of $N^\star$ whose interaction graph is $G=(V,E)$ such that $\mathcal{N}_o = V = \{o,1,2,3,4\}$. The* transfer matrix *$M$ associated with N is the matrix of order $2^{|\mathcal{N}_o^*|}$ whose coefficients are those of the following linear system of projective and conditional equations in which the unknowns are*

but may have importance in the context of simulations because of the impossibility to simulate the dynamical behaviours of infinite NSBANs. In this case, focusing on a central automaton of N^∞ is relevant in the sense that it is the farthest from the boundary on average and is as a consequence a priori amongst the automata that are the less influenced by the boundary instances.

the μ's:

$$
\begin{cases}
\mu([\{1,2,3,4\},\emptyset]) + \mu([\{2,3,4\},\{1\}]) & = & \mu([\{2,3,4\},\emptyset]) \\
\mu([\{1,2,3,4\},\emptyset]) + \mu([\{1,3,4\},\{2\}]) & = & \mu([\{1,3,4\},\emptyset]) \\
\mu([\{1,2,3,4\},\emptyset]) + \mu([\{1,2,4\},\{3\}]) & = & \mu([\{1,2,4\},\emptyset]) \\
\mu([\{1,2,3,4\},\emptyset]) + \mu([\{1,2,3\},\{4\}]) & = & \mu([\{1,2,3\},\emptyset]) \\
\mu([\{2,3,4\},\{1\}]) + \mu([\{3,4\},\{1,2\}]) & = & \mu([\{3,4\},\{1\}]) \\
\mu([\{2,3,4\},\{1\}]) + \mu([\{2,4\},\{1,3\}]) & = & \mu([\{2,4\},\{1\}]) \\
\mu([\{2,3,4\},\{1\}]) + \mu([\{2,3\},\{1,4\}]) & = & \mu([\{2,3\},\{1\}]) \\
\mu([\{1,3,4\},\{2\}]) + \mu([\{1,4\},\{2,3\}]) & = & \mu([\{1,4\},\{2\}]) \\
\mu([\{1,3,4\},\{2\}]) + \mu([\{1,3\},\{2,4\}]) & = & \mu([\{1,3\},\{2\}]) \\
\mu([\{1,2,4\},\{3\}]) + \mu([\{1,2\},\{3,4\}]) & = & \mu([\{1,2\},\{3\}]) \\
\mu([\{3,4\},\{1,2\}]) + \mu([\{4\},\{1,2,3\}]) & = & \mu([\{4\},\{1,2\}]) \\
\mu([\{3,4\},\{1,2\}]) + \mu([\{3\},\{1,2,4\}]) & = & \mu([\{3\},\{1,2\}]) \\
\mu([\{2,4\},\{1,3\}]) + \mu([\{2\},\{1,3,4\}]) & = & \mu([\{2\},\{1,3\}]) \\
\mu([\{1,4\},\{2,3\}]) + \mu([\{1\},\{2,3,4\}]) & = & \mu([\{1\},\{2,3\}]) \\
\mu([\{4\},\{1,2,3\}]) + \mu([\emptyset,\{1,2,3,4\}]) & = & \mu([\emptyset,\{1,2,3\}]) \\
\sum_{[A,B]\in\{0,1\}^{|\mathcal{N}_o^*|}} \Phi_o(A,B)\cdot\mu([A,B]) & = & \mu([\{o\},\emptyset])
\end{cases}. \tag{4}
$$

From Definition 2 and Equation 4, we derive:

$$
M = \begin{array}{c}
\left(\begin{array}{c|cccc|cccccc|cccc|c}
\mathbf{1} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\mathbf{1} & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\mathbf{1} & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \mathbf{1} & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \mathbf{1} & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & \mathbf{1}
\end{array}\right) \\
\begin{array}{c|c|c|c|c}
\Phi_4 & \qquad\Phi_3\qquad & \qquad\qquad\Phi_2\qquad\qquad & \qquad\Phi_1\qquad & \Phi_0
\end{array}
\end{array},
$$

where: $\Phi_4 = \frac{e^{u_0+4u_1+\eta_o^k(\mathcal{N}_o)}}{1+e^{u_0+4u_1+\eta_o^k(\mathcal{N}_o)}}$, $\Phi_3 = \frac{e^{u_0+3u_1+\eta_o^k(A)}}{1+e^{u_0+3u_1+\eta_o^k(A)}}$ (with $|A| = 3$), $\Phi_2 = \frac{e^{u_0+2u_1+\eta_o^k(A)}}{1+e^{u_0+2u_1+\eta_o^k(A)}}$ (with $|A| = 2$), $\Phi_1 = \frac{e^{u_0+u_1+\eta_o^k(A)}}{1+e^{u_0+u_1+\eta_o^k(A)}}$ (with $|A| = 1$) and $\Phi_0 = \frac{e^{u_0}}{1+e^{u_0}}$.

4 Boundary sensitivity of attractive NSBANs – Theory

As evoked above, $N^\star$ is boundary sensitive if and only if two different instances of its covering system $\mathcal{S}$ admit distinct invariant measures. For the latter statement to hold, structural parameters that characterise the system instances have to be intimately related [18, 39]. From a more local point of view, for $N^\star$ to be boundary sensitive, this invariant measure non-uniqueness needs to be retrieved at the level of the stationary probability of central automaton o. Now, the transfer matrix M above characterises the asymptotic dynamical behaviour of o. From the previous lines, it is easy to derive that a linear dependency between projective and conditional equations of the linear system of Equation 4 is necessary for o to behave asymptotically differently when subjected to two distinct instances of the system $\mathcal{S}$ covering $N^\star$. So, *we are going to prove a necessary and sufficient condition on* NSBAN*s that validates the nullity of the determinant of their transfer matrices.*

In [10], Demongeot analysed some properties of Markov random fields and obtained a general formula characterising the nullity of the determinants of transfer matrices like those described above. That resulted in the following lemma of which we will make a specific use.

Lemma 1. *The nullity of the determinant of the transfer matrix M is characterised by:*

$$\mathrm{Det}M = 0 \iff \sum_{K \subseteq \mathcal{N}_o^*} (-1)^{|\mathcal{N}_o^* \setminus K|} \cdot \Phi_o(K, \mathcal{N}_o^* \setminus K) = 0.$$

Notice that Lemma 1 is dived into the general framework of random fields and gives no precisions about structural conditions of phase transitions in our context. Nevertheless, on its basis, we derive another characterisation of the nullity of Det$M$ that makes sense for NSBANs.

Definition 3. *Let N be an attractive* NSBAN *of order k in $\mathbb{Z}^2$ and let i be an arbitrary automaton of N. The non-linear term of i, denoted by η_i^k, is* symmetric *if and only if:*

$$\forall K \subseteq \mathcal{N}_i^*,\ \eta_i^k(\mathcal{N}_i^*) = \eta_i^k(K) + \eta_i^k(\mathcal{N}_i^* \setminus K).$$

Notice that the choice of this symmetry condition directly comes from the linear dependency of projective and conditional equations of Equation 4 induced by the nullity of Det$M$. More precisely, this linear dependency means that there exists a specific relation between the interaction potentials u's that define N. As shown in [13, 40] in the context of LSBANs, this peculiar relation is a counter-balancing relation between negative singleton potentials and positive couple potentials. From this knowledge, it seemed natural that the same kind of counter-balancing relation occurs in NSBANs. Now, remark that the symmetry of the non-linear term constitutes a way to build non-linear interaction potentials of different signs in order to favour the counter-balancing effect.

Let us prove that a particular case of the non-linear symmetry is necessary and sufficient for Det$M = 0$ to hold. To do so, let us begin by studying properties of the general symmetric non-linear term. In the sequel, let us consider that, for any $K \subseteq \mathcal{N}_o^*$, the non-linear term $\eta_o^k(K)$ is symmetric and equals $-2u_0 - \sum_{j \in \mathcal{N}_o^*} u_1 - \eta_o^k(\mathcal{N}_o^* \setminus K)$. First, Lemma 2 gives a characterisation of the symmetric non-linear term.

Lemma 2. *Let N be an attractive* NSBAN *of order k in $\mathbb{Z}^2$. Given an arbitrary $K \subseteq \mathcal{N}_o^*$ and the non-linear term on K defined by $\eta_o^k(K) = -2u_0 - \sum_{j \in \mathcal{N}_o^*} u_1 - \eta_o^k(\mathcal{N}_o^* \setminus K)$, the symmetry property of the non-linear term of N verifies:*

$$\forall K \subseteq \mathcal{N}_o^*,\ \eta_o^k(K) = \eta_o^k(\mathcal{N}_o^*) - \eta_o^k(\mathcal{N}_o^* \setminus K) \iff u_0 + \frac{\sum_{j \in \mathcal{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = 0. \quad (5)$$

Proof. Denoting $\eta_o^k(\mathcal{N}_o^*) - \eta_o^k(\mathcal{N}_o^* \setminus K)$ by η_{sym} and developing the left member of Equation 5 by definition of the non-linear term, trivially, we have:

$$\begin{aligned}
\forall K \subseteq \mathcal{N}_o^*,\ \eta_o^k(K) = \eta_{\mathrm{sym}} &\iff -2u_0 - \sum_{j \in \mathcal{N}_o^*} u_1 - \eta_o^k(\mathcal{N}_o^* \setminus K) = \eta_{\mathrm{sym}} \\
&\iff -2u_0 - \sum_{j \in \mathcal{N}_o^*} u_1 = \eta_o^k(\mathcal{N}_o^*) \\
&\iff u_0 + \frac{\sum_{j \in \mathcal{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = 0.
\end{aligned}$$

□

Now, let us express the symmetric property of the non-linear term by means of the conditional probabilities Φ_o's.

Lemma 3. *Let N be an attractive* NSBAN *of order k in $\mathbb{Z}^2$. Then, the following equation holds:*

$$\forall K \subseteq \mathcal{N}_o^*,\ u_0 + \frac{\sum_{j\in\mathcal{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = 0 \iff \Phi_o(K, \mathcal{N}_o^* \setminus K) + \Phi_o(\mathcal{N}_o^* \setminus K, K) = 1. \quad (6)$$

Proof. The proof is made directly by expanding and then simplifying the right member of Equation 6. First, we have:

$$\begin{aligned}
&\forall K \subseteq \mathcal{N}_o^*,\ \Phi_o(K, \mathcal{N}_o^* \setminus K) + \Phi_o(\mathcal{N}_o^* \setminus K, K) = 1\\
\iff\ & \frac{e^{u_0+\sum_{j\in K} u_1+\eta_o^k(K)}}{1+e^{u_0+\sum_{j\in K} u_1+\eta_o^k(K)}} + \frac{e^{u_0+\sum_{j\in\mathcal{N}_o^*\setminus K} u_1+\eta_o^k(\mathcal{N}_o^*\setminus K)}}{1+e^{u_0+\sum_{j\in\mathcal{N}_o^*\setminus K} u_1+\eta_o^k(\mathcal{N}_o^*\setminus K)}} = 1\\
\iff\ & \frac{e^{u_0+\sum_{j\in\mathcal{N}_o^*\setminus K} u_1+\eta_o^k(\mathcal{N}_o^*\setminus K)}}{1+e^{u_0+\sum_{j\in\mathcal{N}_o^*\setminus K} u_1+\eta_o^k(\mathcal{N}_o^*\setminus K)}} = 1 - \frac{e^{u_0+\sum_{j\in K} u_1+\eta_o^k(K)}}{1+e^{u_0+\sum_{j\in K} u_1+\eta_o^k(K)}}\\
\iff\ & \frac{e^{u_0+\sum_{j\in\mathcal{N}_o^*\setminus K} u_1+\eta_o^k(\mathcal{N}_o^*\setminus K)}}{1+e^{u_0+\sum_{j\in\mathcal{N}_o^*\setminus K} u_1+\eta_o^k(\mathcal{N}_o^*\setminus K)}} = \frac{e^{-u_0-\sum_{j\in K} u_1-\eta_o^k(K)}}{1+e^{-u_0-\sum_{j\in K} u_1-\eta_o^k(K)}}.
\end{aligned}$$

Consider this last equation. In order to ease the reading, let us do the following change of variable: let ν_ℓ and ν_r (resp. δ_ℓ and δ_r) be respectively the numerators (resp. the denominators) of the left and right members. Furthermore, let $\kappa = e^{\sum_{j\in\mathcal{N}_o^*\setminus K} u_1-\sum_{j\in K} u_1-\eta_o^k(K)+\eta_o^k(\mathcal{N}_o^*\setminus K)}$. Then, we have:

$$\begin{aligned}
&\forall K \subseteq \mathcal{N}_o^*,\ \Phi_o(K, \mathcal{N}_o^* \setminus K) + \Phi_o(\mathcal{N}_o^* \setminus K, K) = 1\\
&\iff \tfrac{\nu_\ell}{\delta_\ell} = \tfrac{\nu_r}{\delta_r} \iff \nu_\ell \cdot \delta_r = \nu_r \cdot \delta_\ell \iff \nu_\ell + \kappa = \nu_r + \kappa\\
&\iff \nu_\ell = \nu_r \iff e^{u_0+\sum_{j\in\mathcal{N}_o^*\setminus K} u_1+\eta_o^k(\mathcal{N}_o^*\setminus K)} = e^{-u_0-\sum_{j\in K} u_1-\eta_o^k(K)}\\
&\iff u_0 + \textstyle\sum_{j\in\mathcal{N}_o^*\setminus K} u_1 + \eta_o^k(\mathcal{N}_o^* \setminus K) = -u_0 - \sum_{j\in K} u_1 - \eta_o^k(K)\\
&\iff \eta_o^k(K) = -2u_0 - \textstyle\sum_{j\in\mathcal{N}_o^*} u_1 - \eta_o^k(\mathcal{N}_o^* \setminus K).
\end{aligned}$$

Now, by the hypothesis of the symmetry of the non-linear term, we have:

$$\forall K \subseteq \mathcal{N}_o^*,\ \Phi_o(K, \mathcal{N}_o^* \setminus K) + \Phi_o(\mathcal{N}_o^* \setminus K, K) = 1 \iff \eta_o^k(K) = \eta_o^k(\mathcal{N}_o^*) - \eta_o^k(\mathcal{N}_o^* \setminus K),$$

and, by Lemma 2, we obtain:

$$\forall K \subseteq \mathcal{N}_o^*,\ \Phi_o(K, \mathcal{N}_o^* \setminus K) + \Phi_o(\mathcal{N}_o^* \setminus K, K) = 1 \iff u_0 + \frac{\sum_{j\in\mathcal{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = 0,$$

which is the expected result. $\square$

Now, we own all the necessary intermediary elements to prove that the symmetry of the non-linear term is sufficient for $\mathrm{Det}M$ to be null. This leads to Proposition 1, which will be made finer later to obtain a characterisation of the structural necessary condition for phase transition to hold.

Proposition 1. *Let N be an attractive* NSBAN *of size n and order k in $\mathbb{Z}^2$. A symmetric non-linear term is sufficient for the nullity of* $\mathrm{Det}M$*:*

$$u_0 + \frac{\sum_{j\in\mathcal{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = 0 \implies \mathrm{Det}M = 0. \tag{7}$$

Proof. First, let us show that the symmetry of the non-linear term is a sufficient condition of the nullity of $\mathrm{Det}M$. From Lemma 1 and because of the parity of the cardinal of $\mathcal{N}_o^*$ (the number of subsets of $\mathcal{N}_o^*$ of even cardinal equals the number of subsets of $\mathcal{N}_o^*$ of odd cardinal), we have:

$$\mathrm{Det}M = 0 \iff \sum_{K\subseteq\mathcal{N}_o^*} (-1)^{|\mathcal{N}_o^*\setminus K|} \cdot \Phi_o(K, \mathcal{N}_o^* \setminus K) = 0$$
$$\iff \sum_{K\subseteq\mathcal{N}_o^*} (-1)^{|\mathcal{N}_o^*\setminus K|} \times \frac{1}{2} \cdot (\Phi_o(K, \mathcal{N}_o^* \setminus K) + \Phi_o(\mathcal{N}_o^* \setminus K, K)) = 0. \tag{8}$$

Then, from Lemma 3, we have:

$$\sum_{K\subseteq\mathcal{N}_o^*} (-1)^{|\mathcal{N}_o^*\setminus K|} \cdot \frac{1}{2} = 0 \implies \mathrm{Det}M = 0.$$

Notice that the previous equation always holds under the general hypothesis of symmetry of the non-linear term of N (see Equation 6). As a result, following Lemmas 1, 2 and 3, we obtain:

$$u_0 + \frac{\sum_{j\in\mathcal{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = 0 \implies \mathrm{Det}M = 0,$$

which is the expected result. $\square$

Now we have succeeded in showing that the symmetry of non-linear terms is sufficient for the nullity of $\mathrm{Det}M$ to hold, let us pursue by showing to what extent it is also a necessary condition. To do so, let us define two new elements that will be useful to reach our goal: the symmetry of the interaction potentials u's, called the *symmetry condition* (cf. Definition 4), and the the compensation between the global potentials of configurations, called the *compensation condition* (cf. Definition 5).

Let $\mathsf{h} = h \circ exp$ be the exponential homographic function defined as $\mathsf{h}(x) : x \mapsto \frac{e^x}{1+e^x}$. From the transfer matrix M (cf. page 13), let us denote the following quantities Q_i which correspond respectively to the exponents of the conditional probabilities Φ_i, *i.e.* the global potentials of a configuration, for $i \in \{0, \ldots, 4\}$, that have to be taken into account in the formula characterising the nullity of Det$M$ in Lemma 1:

$$
\begin{aligned}
Q_0 &= u_0, \\
Q_1 &= u_0 + u_1 + u_2, \\
Q_2 &= u_0 + 2u_1 + 3u_2 + u_3, \\
Q_3 &= u_0 + 3u_1 + 6u_2 + 4u_3 + u_4, \\
Q_4 &= u_0 + 4u_1 + 10u_2 + 10u_3 + 5u_4 + u_5.
\end{aligned}
$$

Moreover, let us use the following notation: $\forall i \in \{0, \ldots, 4\}, \mathsf{g}(Q_i, Q_{4-i}) = \mathsf{h}(Q_i) + \mathsf{h}(Q_{4-i})$.

Definition 4. *The* symmetry condition*, based on the interaction potentials u's, is given by:*

$$Q_0 + Q_4 = 0, Q_1 + Q_3 = 0 \text{ and } Q_2 = 0.$$

From this definition of symmetry, we will see in Lemma 4 a characterisation of this condition which is the generalisation of the Ruelle's condition [39] of phase transition as it appears in Proposition 1.

Lemma 4. *We have the following equivalence that relates the symmetry condition to the interaction potentials:*

$$Q_0 + Q_4 = 0, Q_1 + Q_3 = 0 \text{ and } Q_2 = 0 \iff u_0 + \frac{\sum_{j \in \mathcal{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = 0.$$

Proof. By definition, we have first that $(Q_0 + Q_4)/2 = u_0 + 2u_1 + \frac{\eta_o^k(\mathcal{N}_o^*)}{2}$. From this, we derive directly that $Q_0 + Q_4 = 0 \iff u_0 + 2u_1 + \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = 0$. Now, let us denote by K_j any subset of the strict activated neighbourhood of the central automaton o of cardinal j. By Definition 3 of the symmetry of the non-linear term and Lemma 2, we can write:

$$3u_2 + u_3 = \eta_o^k(K_2) = \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = -u_0 - 2u_1$$

that implies that $Q_2 = 0$ and, similarly:

$$7u_2 + 4u_3 + u_4 = \eta_o^k(K_1) + \eta_o^k(K_3) = \eta_o^k(\mathcal{N}_o^*) = -2u_0 - 4u_1$$

that implies that $Q_1 + Q_3 = 0$, which is the expected result. □

Notice that Lemma 4 emphasises the counter-balancing effect between global potentials of complementary configurations of the neighbourhood of the central automaton, as mentioned above at page 15.

Definition 5. *The* compensation condition *is given by:*

$$Q_2 = \frac{Q_0 + Q_4}{2} = \frac{Q_1 + Q_3}{2}.$$

We will use in the sequel a weaker notion, named the *half compensation condition*, defined as: $Q_2 = \frac{Q_0+Q_4}{2}$ or $Q_2 = \frac{Q_1+Q_3}{2}$. From this, let us prove that the symmetry condition is sufficient for having both the nullity of $\mathrm{Det}M$ and the half compensation condition.

Lemma 5. *The symmetry condition implies both* $\mathrm{Det}M$ *nullity and the half compensation condition. Formally, we have:*

$$Q_0 + Q_4 = 0, Q_1 + Q_3 = 0 \text{ and } Q_2 = 0$$
$$\implies Q_2 = 0,\ \mathrm{Det}M = 0 \text{ and } Q_2 = \frac{Q_0 + Q_4}{2}.$$

Proof. From Proposition 1 and Lemma 4, it is direct that the symmetry condition is sufficient for the nullity of $\mathrm{Det}M$. Furthermore, notice that under the hypothesis of the symmetry condition, we have $Q_2 = 0$ and $Q_0 + Q_4 = 0$. As a consequence, we get the half compensation condition: $\frac{Q_0+Q_4}{2} = Q_2$. □

Lemma 6 below presents a relation between the half compensation condition and the compensation condition through the nullity of $\mathrm{Det}M$.

Lemma 6.

$$Q_2 = 0,\ \mathrm{Det}M = 0 \text{ and } Q_2 = \frac{Q_0 + Q_4}{2}$$
$$\implies Q_2 = 0 \text{ and } \frac{Q_0 + Q_4}{2} = Q_2 = \frac{Q_1 + Q_3}{2}.$$

Proof. Let us consider the expansion of $\mathrm{Det}M = 0$. We have:

$$\begin{aligned}
\mathrm{Det}M = 0 &\implies \mathsf{g}(Q_0, Q_4) + 6\mathsf{h}(Q_2) - 4(\mathsf{g}(Q_1, Q_3)) = 0 \\
&\implies (\mathsf{g}(Q_0, Q_4) - 2\mathsf{h}(Q_2)) - 4(\mathsf{g}(Q_1, Q_3) - 2\mathsf{h}(Q_2)) = 0 \\
&\implies (\frac{\mathsf{g}(Q_0, Q_4)}{2} - \mathsf{h}(Q_2)) - 4(\frac{\mathsf{g}(Q_1, Q_3)}{2} - \mathsf{h}(Q_2)) = 0 \qquad (9) \\
&\implies (\frac{\mathsf{g}(Q_0, Q_4)}{2} - \mathsf{h}(Q_2)) - 4(\frac{\mathsf{g}(Q_1, Q_3)}{2} - \mathsf{h}(Q_2)) = 0
\end{aligned}$$

Furthermore, consider the Jensen's inequalities that can be generalised in the case of a sigmoid function f symmetric with respect to its inflection point by:

$$\mathsf{sgn}(\frac{x+y}{2}) \times \frac{f(x)+f(y)}{2} \leq \mathsf{sgn}(\frac{x+y}{2}) \times f(\frac{x+y}{2}),$$

the equality being possible only if $x + y = 0$. In our case, because h is a sigmoid function symmetric with respect to its inflection point, we can write:

$$\begin{aligned}
&\forall i \in \{0, \ldots, 4\}, \\
&\mathsf{sgn}(\frac{Q_i + Q_{4-i}}{2}) \times \frac{\mathsf{h}(Q_i) + \mathsf{h}(Q_{4-i})}{2} \leq \mathsf{sgn}(\frac{Q_i + Q_{4-i}}{2}) \times \mathsf{h}(\frac{Q_i + Q_{4-i}}{2}).
\end{aligned}$$

Now, by hypothesis of the half compensation condition $\frac{Q_0+Q_4}{2} = Q_2$ and because $Q_2 = 0$ (due the symmetry condition), we have:

$$\frac{\mathsf{g}(Q_0, Q_4)}{2} = \mathsf{h}(Q_2).$$

Thus, following Equation 9, $\frac{\mathsf{g}(Q_1,Q_3)}{2} - \mathsf{h}(Q_2) = 0$. And, since $Q_2 = 0$ by hypothesis, Q_2 is the barycentre of (Q_1, Q_3) such that $\frac{Q_1+Q_3}{2} = Q_2$, and we get the expected result. □

Lemma 7 below shows that the compensation condition associated with $Q_2 = 0$ implies the symmetry condition. The proof is the direct consequence of the instanciation of $Q_2 = 0$ in the symmetry condition.

Lemma 7.

$$\begin{aligned}
&Q_2 = \frac{Q_0 + Q_4}{2} = \frac{Q_1 + Q_3}{2} \ \textit{and}\ Q_2 = 0 \\
&\qquad\qquad \implies Q_0 + Q_4 = 0,\ Q_1 + Q_3 = 0 \ \textit{and}\ Q_2 = 0.
\end{aligned}$$

From Proposition 1 and Lemmas 4, 5, 6 and 7, we get the expected Theorem 4 that characterises the nullity of Det$M$ from the symmetry condition.

Theorem 4.

$$\begin{aligned}
&Q_0 + Q_4 = 0, Q_1 + Q_3 = 0 \textit{ and } Q_2 = 0\\
&\qquad\qquad \implies Q_2 = 0,\ \mathrm{Det}M = 0 \textit{ and } Q_2 = \frac{Q_0 + Q_4}{2}\\
&\qquad\qquad \implies Q_2 = 0 \textit{ and } \frac{Q_0 + Q_4}{2} = Q_2 = \frac{Q_1 + Q_3}{2}\\
&\qquad\qquad\qquad\qquad \implies Q_0 + Q_4 = 0,\ Q_1 + Q_3 = 0 \textit{ and } Q_2 = 0.
\end{aligned}$$

5 Boundary sensitivity of attractive NSBANs – Simulations

In order to illustrate this family of NSBANs sensitive to their boundary and to empirically check the sufficiency of the condition obtained, we have performed numerical simulations. The general idea has been to consider two dimensional BANs dived into squared lattices, of increasing sizes. The measure that has been taken into account, denoted by S and called dissimilarity measure, consists in computing asymptotically the difference of the activity of their central automata (*i.e.*, the number of asymptotic time steps during which central automata are in state 1) when NSBANs are subjected to two distinct boundary instances. The details of the simulation protocol are presented in [15]. Figure 3 pictures the results obtained on the family of NSBANs of order $k = 3$, that is the family considering singleton, couple and triplet interaction potentials with coalitions of pairs of cells.

More precisely, considered NSBANs have been subjected to the following boundary instances: $\circ = (0, \dots, 0)$ and $\bullet = (1, \dots, 1)$. This choice comes from results obtained in [5] that show that they are those that induce the maximal influence on the behaviour of attractive NSBANs of order $k \leq 2$. The dissimilarity measure presented is the average of five dissimilarity measures obtained from five distinct simulations (with different initial conditions) of the dynamical behaviours of 20 000 NSBANs of order 3 of respective sizes 11×11, 37×37 and 131×131. The number of steps employed to let every NSBAN evolve to its equilibrium has been fixed to 10 000 and dissimilarity measure S has been computed on the 1 000 following time steps. Notice that every couple of values on the plane $(0, u_1, u_2)$ corresponds to one NSBAN defined according to parameters $u_0 = 0$, $0 \leq u_1 \leq 20$ and $-10 \leq u_2 \leq 0$ with a

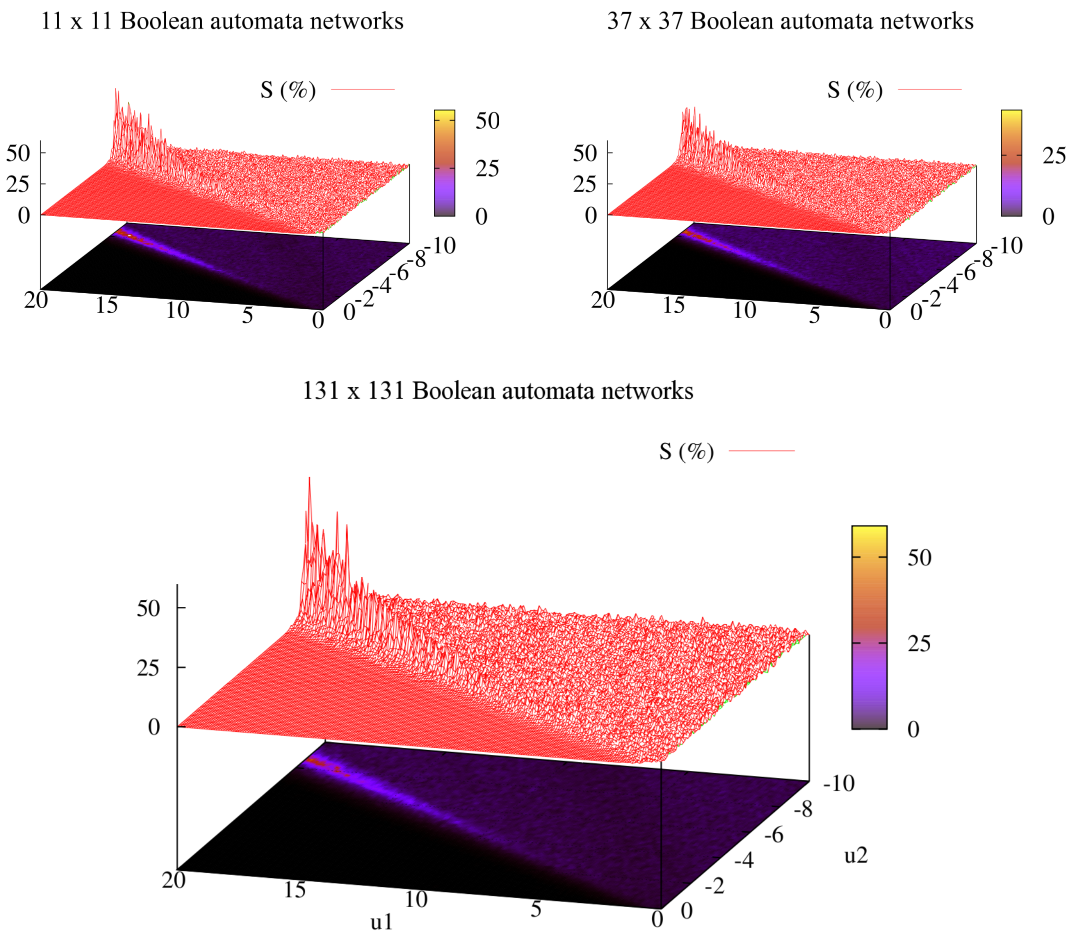

Figure 3: Emerging phase transitions in NSBANs of order 3 on the straightline $2u_1 + 5u_2 = 0$.

variation step equal to 0.1. The lattice sizes chosen allow to obtain results on BANs of three different orders of magnitude, which supports the pertinence of the results. In particular, for any size, the dissimilarity measures that are significantly strictly positive are located on the straightline of equation $2u_1 + 5u_2 = 0$, which corresponds to what has been obtained theoretically. Indeed, for NSBANs of order 3, the generalised Ruelle's condition related to the nullity of Det$M$ is:

$$u_0 + \frac{\sum_{j\in\mathcal{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = 0 \iff u_0 + \frac{4u_1}{2} + \frac{\binom{5}{2}u_2}{2} = 0$$
$$\iff u_0 + 2u_1 + 5u_2 = 0,$$

which gives

$$2u_1 + 5u_2 = 0$$

as illustrated in Figure 3 when $u_0 = 0$. Moreover, by considering the following global interaction potentials Q_0 and Q_4, to which are applied the symmetry and the compensation conditions detailed above and the nullity of u_0, u_3, u_4 and u_5, we get $2u_1 + 5u_2 = 0$ which supports the previous result.
As a consequence, the results obtained with simulations emphasise that the parametric equation of the nullity of the transfer matrix determinant is also a sufficient condition. Indeed, although there exists on the straightline $2u_1+5u_2 = 0$ (reduced to the plan of attractive NSBANs) values of parameters where the dissimilarity measure is weak, this line clearly shows a frontier between two domains in the phase space, one with $S = 0$ and another noisy one with $S \approx 0$.

6 Conclusion

This paper aimed at addressing the problem of the emergence of phase transitions due to the influence of boundaries in the dynamical behaviour of attractive NSBANs on $\mathbb{Z}^2$. With this work, we have generalised existing results, notably by exploiting on NSBANs the knowledge already owned on LSBANs.

Theoretical questions that stay open, or those that have been highlighted in this study, are numerous. Of course, the problem of the characterisation of the domain of phase transition remains open although it has been addressed pertinently here in the attractive case. Also, the case of repulsive NSBANs, in which the strict neighbourhood interaction potentials are negative, has not been studied for now. Except this, we think that the most ambitious and interesting work for the future would be to become progressively closer to the biological reality. While BANs on $\mathbb{Z}^2$ present undeniable advantages to lead such a study, to relax step by step their inherent constraints could allow to obtain new insights about the behaviour of biological interacting systems. The constraint that seems to be the first to be removed is the functional translation invariance (by preserving the global translation invariance on lattices). The idea would be to make interaction potentials as functions of the interaction weights but also of the distance of automata to the centre of the network. Another aspect that opens interesting properties is the loss of the synchronism imposed by the parallel updating mode used here. Being given the difficulties underlying the notion of boundary sensitivity, it is certain that combining it with that of structural robustness (in the sense of Thom [42], whose objective is to understand the impact of changes of global transition functions on the dynamical behaviours of dynamical systems) dealt with variations of updating modes is indisputably a long term project. However, it is a necessary step if we expect fundamental general results biologically practical.

From the application point of view, the results obtained have shown that the information provided by the environment of a network is effectively broadcast throughout the whole network, even when the network is arbitrarily large. This suggests that the boundaries play a significant role in systems, and not only in those that are “regular”. Consequently, any study in a modelling context should address the problem of the impact of the boundary before changing its underlying abstraction level. This work could also have direct applications in the classical framework formal neural networks and their associative memory and learning properties [24, 33], where boundaries could perturb or facilitate these two phases of memorisation and restitution by computation. Thus, it would be interesting to identify boundaries allowing and boundaries avoiding expected associations. Eventually, non-linearity itself could be at the center of further works. As it has been evoked, it gives a mean to integrate cooperative and competitive coalitions without increasing problem sizes, which is a major parameter when we attempt to characterise the dynamical behaviour of regulation networks. So, in the context of automata networks viewed as models of “real” genetic regulation networks, to succeed in formally describing the conditions under which the use of non-linear functions rather than the adding of new vertices in the architecture of networks could constitute a relevant benefits for theoretical bio-informatics.

7 Acknowledgements

This work has been partially supported by the project SYNBIOTIC (ANR-2010-BLAN-030701) and the project FRI (PACA-2015_01134).

References

[1] D. H. Ackley, G. E. Hinton, and T. J. Sejnowski. A learning algorithm for Boltzmann machines. *Cognitive Science*, 9:147–169, 1985.

[2] P. Aloy, B. Böttcher, H. Ceulemans, C. Leutwein, C. Mellwig, S. Fischer, A. C. Gavin, P. Bork, G. Superti-Furga, L. Serrano, and R. B. Russel. Structure-based assembly of protein complexes in yeast. *Science*, 303:2026–2029, 2004.

[3] C. A. Anastassiou, S. M. Montgomery, M. Barahona, G. Buzsáki, and C. Koch. The effect of spatially inhomogeneous extracellular electric fields on neurons. *The Journal of Neuroscience*, 30:1925–1936, 2010.

[4] J. Aracena, M. González, A. Zuñiga, M. A. Mendez, and V. Cambiazo. Regulatory network for cell shape changes during drosophila ventral furrow formation. *Journal of Theoretical Biology*, 239:49–62, 2006.

[5] H. Ben Amor, J. Demongeot, and S. Sené. Structural sensitivity of neural and genetic networks. In *Proceedings of MICAI*, volume 5317 of *Lecture Notes in Computer Science*, pages 973–986. Springer, 2008.

[6] C. Berge. *Graphes et hypergraphes*. Dunod, 1973.

[7] N. E. Buchler, U. Gerland, and T. Hwa. Nonlinear protein degradation and the function of genetic circuits. *Proceedings of the National Academy of Sciences of the USA*, 102:9559–9564, 2004.

[8] M. Cosnard and E. Goles. Discrete state neural networks and energies. *Neural Networks*, 10:327–334, 1997.

[9] M. Cosnard, P. Koiran, and H. Paugam-Moisy. Complexity issues in neural network computations. In *Proceedings of LATIN*, volume 583 of *Lecture Notes in Computer Science*, pages 530–544. Springer, 1992.

[10] J. Demongeot. Asymptotic inference for Markov random field on $\mathbb{Z}^d$. *Springer Series in Synergetics*, 9:254–267, 1981.

[11] J. Demongeot, E. Goles, M. Morvan, M. Noual, and S. Sené. Attraction basins as gauges of the robustness against boundary conditions in biological complex systems. *PLoS One*, 5:e11793, 2010.

[12] J. Demongeot, O. Hansen, and C. Taramasco. Complex systems and contagious social diseases: the example of obesity. *Virulence*, 7:129–140, 2015.

[13] J Demongeot, C. Jézéquel, and S. Sené. Boundary conditions and phase transitions in neural networks. Theoretical results. *Neural Networks*, 21:971–979, 2008.

[14] J. Demongeot and S. Sené. Boundary conditions and phase transitions in neural networks. Simulation results. *Neural Networks*, 21:962–970, 2008.

[15] J. Demongeot and S. Sené. The singular power of the environment on stochastic nonlinear threshold Boolean automata networks. In *Proceedings of CMSB*, pages 55–64. ACM, 2011.

[16] J. Demongeot and C. Taramasco. Evolution of social networks: the example of obesity. *Biogerontology*, 15:611–626, 2014.

[17] R. L. Dobrushin. Gibbsian random fields for lattice systems with pairwise interactions. *Functional Analysis and its Applications*, 2:292–301, 1968.

[18] R. L. Dobrushin. The problem of uniqueness of a Gibbsian random field and the problem of phase transitions. *Functional Analysis and its Applications*, 2:302–312, 1968.

[19] E. Goles and S. Martínez. *Neural and Automata Networks: Dynamical Behavior and Applications*. Kluwer Academic Publishers, 1990.

[20] E. Goles and J. Olivos. Periodic behaviour of generalized threshold functions. *Discrete Mathematics*, 30:187–189, 1980.

[21] E. Goles-Chacc, F. Fogelman-Soulie, and D. Pellegrin. Decreasing energy functions as a tool for studying threshold networks. *Discrete Applied Mathematics*, 12:261–277, 1985.

[22] F. Harary. *Graph Theory*. Addison-Wesley, 1969.

[23] G. E. Hinton and T. J. Sejnowski. *Parallel Distributed Processing: Explorations in the Microstructure of Cognition*, volume 1, chapter Learning and relearning in Boltzmann machines, pages 282–317. MIT Press, 1986.

[24] J. J. Hopfield. Neural networks and physical systems with emergent collective computational abilities. *Proceedings of the National Academy of Sciences of the USA*, 79:2554–2558, 1982.

[25] 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*, 81:3088–3092, 1984.

[26] E. Ising. Beitrag zur theorie des ferromagnetismus. *Zeitschrift für Physik A. Hadrons and Nuclei*, 31:253–258, 1925.

[27] M. U. Kaikkonen, M. T. Y. Lam, and Glass C. K. Non-coding RNAs as regulators of gene expression and epigenetics. *Cardiovascular Research*, 90:430–440, 2011.

[28] S. A. Kauffman. Homeostasis and differentiation in random genetic control networks. *Nature*, 224:177–178, 1969.

[29] S. A. Kauffman. Metabolic stability and epigenesis in randomly constructed genetic nets. *Journal of Theoretical Biology*, 22:437–467, 1969.

[30] S. A. Kauffman. *Current Topics in Developmental Biology*, volume 6, chapter Gene regulation networks: a theory for their global structures and behaviors, pages 145–181. Elsevier, 1971.

[31] W. S. McCulloch and W. Pitts. A logical calculus of the ideas immanent in nervous activity. *Journal of Mathematical Biophysics*, 5:115–133, 1943.

[32] L. Mendoza and E. R. Alvarez-Buylla. Dynamics of the genetic regulatory network for *Arabidopsis thaliana* flower morphogenesis. *Journal of Theoretical Biology*, 193:307–319, 1998.

[33] M. Minsky and S. Papert. *Perceptrons: An Introduction to Computational Geometry.* MIT Press, 1969.

[34] L. Onsager. Crystal statistics I. A two dimensional model with an order-disorder. *Physical Review*, 65:117–149, 1944.

[35] Y. Qin and Z.R. Yang. Critical dynamics of the kinetic Ising model with triplet interaction on Sierpinski-gasket-type fractals. *Physical review B.*, 46:11284–11289, 1992.

[36] É. Remy, P. Ruet, and D. Thieffry. Graphic requirements for multistability and attractive cycles in a Boolean dynamical framework. *Advances in Applied Mathematics*, 41:335–350, 2008.

[37] F. Robert. *Discrete Iterations: a Metric Study*, volume 6 of *Springer Series in Computational Mathematics*. Springer, 1986.

[38] D. Ruelle. Statistical mechanics of a one-dimensional lattice gas. *Communications in Mathematical Physics*, 9:267–278, 1968.

[39] D. Ruelle. *Statistical Mechanics: Rigourous Results*. W. A. Benjamin, 1969.

[40] S. Sené. *Influence des conditions de bord dans les réseaux d'automates booléens à seuil et application à la biologie*. PhD thesis, Université Grenoble 1 – Joseph Fourier, 2008.

[41] D. Thieffry and R. Thomas. Dynamical behaviour of biological regulatory networks – II. Immunity control in bacteriophage lambda. *Bulletin of Mathematical Biology*, 57:277–297, 1995.

[42] R. Thom. *Structural Stability and Morphogenesis*. W. A. Benjamin, 1975.

[43] R. Thomas. Boolean formalisation of genetic control circuits. *Journal of Theoretical Biology*, 42:563–585, 1973.

[44] 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*, volume 9 of *Springer Series in Synergetics*, pages 180–193. Springer, 1981.

[45] J. von Neumann. *Theory of Self-Reproducing Automata*. University of Illinois Press, 1966. edited and completed by A. W. Burks.

[46] F.Y. Wu. Rigorous results on the triangular Ising model with pair and tripletinteractions. *Physics Letters A*, 153:73–75, 1991.

[47] X.N. Wu and F.Y. Wu. Exact results for lattice models with pair and triplet interactions. *Journal of Physics A: Mathematical and general*, 22:L1031, 1989.