A necessary condition for boundary sensitivity of attractive non-linear stochastic cellular automata in $\mathbb{Z}^2$

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This paper tackles the question of the environmental robustness of a particular class of two-dimensional finite threshold Boolean cellular automata when they are subjected to distinct fixed boundary instances. More precisely, focusing on a non-linear stochastic version of the classical threshold function governing the evolution of formal neural networks, we show the existence of a necessary condition under which attractive cellular automata of this form become boundary sensitive, *i.e.*, we highlight a condition without which a cellular automaton hits the same asymptotic dynamical behaviour whatever its boundary conditions are. To go further, we give an explicit formula for this necessary condition.
Keywords. Stochastic threshold Boolean cellular automata, non-linear transition functions, boundary sensitivity.

1 Introduction

The theoretical question of the influence of the environment on a system composed of interacting elements over time was born in the domain of mathematical physics in the 1960's. On the basis of the work of Ising on ferromagnetism [13], many researches relating lattice models and their environmental characteristics have been led. Among the most known are surely those of Dobrushin [8, 9] and Ruelle [16, 17] which presented the first results emphasising that the Ising model embedded into a square lattice admits a phase transition depending on the nature of its boundary conditions. Nevertheless, although they come from physics, 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 can help represent external electric fields in a neural context, the post-transcriptional actions of non-coding RNAs in a genetic context, and hormone flows in both of these.

In this paper, despite our interest in the biological applications, the focus is put on a theoretical analysis of the asymptotic dynamical behaviours of a specific class of cellular automata (CAs for short) on $\mathbb{Z}^2$ when the latter are subjected to the influences of distinct boundary instances. Previous works on *linear* stochastic threshold Boolean CAs [5, 6] have shown that the boundary sensitivity of such CAs is very similar to that of the Ising model. In these lines and on the grounds of preliminary results [7], the contribution of this paper is to finally give the explicit formula that characterises a necessary condition according to which *non-linear stochastic threshold Boolean cellular automata* (NSCAs for short) become sensitive to changes of their boundary instances. There also, our interest in non-linearity comes from both the theory and the applications. Indeed, non-linearity constitutes an original way to model coalitions. It allows to represent for instance neurons grouping due to dynamical connections [10] and protein complexes [2] inside transition functions rather than modifying the structural features of networks by adding vertices

Submitted to:
Automata 2012

and edges to their underlying interaction graphs. Thus, it is a mean to introduce synergetic or competitive coalitions without increasing problems sizes (*i.e.*, the sizes of their inputs).

First, in Section 2, we give the main definitions and notations used throughout the paper. After that, we develop the intermediary results that lead to the the explicit formula characterising the condition that is necessary for NSCAs to be sensitive against their boundary instances. Then, a discussion highlighting perspectives of this work concludes the paper.

2 Preliminary definitions and notations

2.1 Structural properties

The *geometric structure* of a finite NSCA N of size n on $\mathbb{Z}^2$ is given by its underlying connected directed graph $G = (V,E)$ (called the *interaction graph* of N), where $V \subseteq \mathbb{Z}^2$ is the set of cells of N (by convention in this paper, cells are numbered from 0 to $n-1$), and $E = \{(i,j) \mid d_{L_1}(i,j) \leq 1\} \subseteq V \times V$ is the set of edges that connect cells of N, where d_{L_1} stands for the L_1 distance. Informally, each cell of V is connected to itself and its nearest cells, which means that N is defined according to the von Neumann neighbourhood. The *complete structure* of N is obtained by associating with every edge $(i,j) \in E$ a label $w_{i,j} \in \mathbb{R}^*$ 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* $\mathscr{N}_i$ of cell i defined as $\mathscr{N}_i = \{j \mid (i,j) \in E\}$ from the *strict neighbourhood* $\mathscr{N}_i^*$ of cell i defined as $\mathscr{N}_i^* = \mathscr{N}_i \setminus \{i\} = \{j \neq i \mid (i,j) \in E\}$. Furthermore, in order for N to be a CA, each cell needs to evolve according to a common transition function. This is ensured by the fact that, in the sequel, every N considered is *totalistic*[1], *translation invariant*[2], such that $\forall i,j \in V,\ \theta_i = \theta_j$, and admits a boundary, whose definition, together with that of the center is given in the next paragraph.

Both the definitions of centre and boundary associated with NSCAs are related to graph theory. The *centre* of a NSCA N is the set of its cells of minimal eccentricity[3]. To define the *boundary* of N, let us consider $V^c = \mathbb{Z}^2 \setminus V$ as the set of vertices that complements V to recover $\mathbb{Z}^2$. The boundary V^{ext} of N is then defined by $V^{\text{ext}} = \{i \in V^c \mid \exists j \in V,\ d_{L_1}(i,j) = 1\}$. From this, we derive that the interaction graph $\mathscr{G} = (\mathscr{V},\mathscr{E})$ of the *system* $\mathscr{S}$ that recovers N and V^{ext} is such that $\mathscr{V} = V \cup V^{\text{ext}}$ and $\mathscr{E} = E \cup \{(i,j) \mid i \in V^{\text{ext}}, j \in V, d_{L_1}(i,j) = 1\}$. With $\mathscr{S}$, we enforce N to be a CA by ensuring that it remains totalistic and translation invariant. That means that $\forall i,j \in V, \forall k \in V^{\text{ext}}, d_{L_1}(i,j) = d_{L_1}(i,k) = 1,\ w_{i,k} = w_{i,j}$. Furthermore, *the states of boundary vertices of V^{ext} remain fixed*. Thus, $\mathscr{S}$ is a system that contains and encloses the finite cellular automaton N.

[1] N is *totalistic* if and only if $\forall i,j,j' \in V,\ j,j' \in \mathscr{N}_i^*,\ w_{i,j} = w_{i,j'}$.

[2] N is *translation invariant* if and only if $\forall i,i' \in V, s = i' - i, \forall j \in \mathscr{N}_i,\ w_{i,j} = w_{i',j+s}$.

[3] 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 not going to i itself 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:

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

2.2 Evolution rule of NSCAs and Markov chains

Since we focus on Boolean CAs, the state x_i of each cell i of N can take values in $\{0,1\}$. Because of the discrete nature of time, abusing language, the state of cell 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 linear stochastic CA that is a generalisation of the Boltzmann machine [1, 12] to the framework of threshold Boolean automata networks. It computes $P(x_i(t+1) = 1 \mid x(t))$, that is the conditional probability for cell i to be at state 1 at time step $t+1$, knowing the states of its neighbours at time t, such that $\forall i \in V, \forall t \in \mathbb{N},\ P(x_i(t+1) = 1 \mid x(t)) = \frac{e^{(\sum_{j \in \mathscr{N}_i} w_{i,j} \cdot x_j(t) - \theta_i)/T}}{1+e^{(\sum_{j \in \mathscr{N}_i} w_{\{i,j\}} \cdot x_j(t) - \theta_i)/T}}$, where θ_i is the *threshold* of i and $T \in \mathbb{R}^+$ is a temperature parameter and allows to make the network studied "more or less probabilistic". When T tends to 0, the transition function above is equivalent to the classical deterministic one [11, 14], except for the value 0 of the exponent of the exponential, for which the choice is not 0, but 1 or 0 with probability $1/2$; when it tends to $+\infty$, the probability for the state of any cell to equal 1 is $1/2$. Without loss of generality, for any cell i of N, its threshold θ_i is made null and its role is played by the auto-interaction weight $w_{i,i}$, which always participates to the computation of the transition function of cell i, whatever the state of the latter. Let us add that this study is restricted to *attractive* stochastic CAs that satisfy $\forall i, j \in V,\ j \in \mathscr{N}_i^*,\ w_{i,j} > 0$, which means that the probability for i to be at state 1 at time $t+1$ knowing the global configuration of the CA at time t increases with the number of its active neighbours.

Let N be a NSCA, with $G = (V,E)$ its interaction graph, and $\mathscr{S}$ its related system associated with graph $\mathscr{G} = (\mathscr{V}, \mathscr{E})$. The evolution of a cell i of N depends on three parameters: $u_{0,i} = w_{i,i}/T$ and $u_{1,\langle i,j \rangle} = w_{i,j}/T$ that represent *linear interaction potentials*, and a function η (see below) that provides the images of *collective interaction potentials* that neighbour cells can activate when several are at state 1 simultaneously. These collective interaction potentials, thus, can take different forms according to the configuration in the neighbourhood of cell i. Let us define and list below the possible interaction potentials which are taken into account:

- 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 $\forall j \in \mathscr{N}_i^*,\ u_{1,i,j} = w_{i,j}/T$;
- the ten *triplet potentials* of i are defined as $\forall j, \ell \in \mathscr{N}_i,\ j \neq \ell,\ u_{2,i,\langle j,\ell \rangle} = w_{i,\langle j,\ell \rangle}/T$ (at least two distinct neighbours of i are at state 1);
- the ten *quadruplet potentials* of i are defined as $\forall j, \ell, m \in \mathscr{N}_i,\ j \neq \ell \neq m,\ u_{3,i,\langle j,\ell,m \rangle} = w_{i,\langle j,\ell,m \rangle}/T$ (at least three distinct neighbours of i are at state 1);
- the five *quintuplet potentials* of i are defined as $\forall j, \ell, m, p \in \mathscr{N}_i,\ j \neq \ell \neq m \neq p,\ u_{4,i,\langle j,\ell,m,p \rangle} = w_{i,\langle j,\ell,m,p \rangle}/T$ (at least four distinct neighbours of i are at state 1);
- the unique *sextuplet potential* is defined as $\forall i, j, \ell, m, p \in \mathscr{N}_i,\ i \neq j \neq \ell \neq m \neq p,\ u_{5,i,\langle i,j,\ell,m,p \rangle} = w_{i,\langle i,j,\ell,m,p \rangle}/T$ (every neighbour of i is at state 1).

Since CAs considered are totalistic and translation invariant, let us right now simplify notations and denote the singleton until 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 cell i receives from a set of neighbour cells j and ℓ. In other words, it represents the interaction potential that the *group* composed of j together with ℓ (viewed as a kind of interacting entity unto itself) has on i. Remark also that interaction

potentials are "cumulative" in the sense that a cell that is subjected to a triplet potential is also subjected to one or two couple potentials (depending on i belonging or not to the group acting on itself) and its singleton potential (which always takes part in the computation of its new state).

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

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

$$\forall i \in V,\ P(x_i(t+1)=1 \mid x(t)) \ = \ f \circ g \circ h_i(x(t)), \tag{1}$$

where $f(y)=\frac{y}{1+y}$, $g(y)=e^y$ and $h_i(x(t))=u_0+\sum_{j\in\mathscr{N}_i^*} u_1 \cdot x_j(t)+\eta_i^k(x(t))$ where $\eta_i^k(x(t))$ is the non-linear term *of N and stands for accounting collective interaction potentials such that:*

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

It follows that NSCAs of order $k=2$ are actually linear 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, we only focus on effective NSCAs of order $3\leq k\leq 6$.

From Equation 1, obviously, the dynamical behaviour of an arbitrary NSCA N of size n (resp. of its associated system $\mathscr{S}$) is a finite *stationary Markov chain* whose random variables are the possible configurations of N (resp. of $\mathscr{S}$) 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. 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 the normalised left eigenvector of a p associated with its eigenvalue 1. A notable fact is that such a μ defines an attractor of C (and consequently of N). Furthermore, by Equation 1, it is obvious that the Markovian matrices of NSCAs 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 $\mathscr{S}$. More precisely, let us consider an *instance* $\mathscr{S}^\circ$ of $\mathscr{S}$ such that the state of each cell of V^{ext} has been fixed to a value in $\{0,1\}$ and denote by μ° its invariant measure. Consider now another distinct instance $\mathscr{S}^\bullet$ of $\mathscr{S}$ and $\mu^\bullet$. Although the invariant measure of N is unique, $\mu^\circ=\mu^\bullet$ does not hold a priori. In [8, 9], Dobrushin characterised phase transitions in the Ising model subjected to boundary instances as domains of structural parameters under which the corresponding Markov chains admit distinct invariant measures. Following the lines drawn by Dobrushin, we say that *a* NSCA *N is* boundary sensitive *and admits a* phase transition *if two different instances of its covering system have distinct invariant measures*. Thus, in the sequel, we propose a method to prove the existence of a structural parametric necessary condition based on the asymptote[4] of NSCAs under which different instances of their covering system lead inevitably to different attractors. Such a condition defines then a domain of phase transitions.

[4]The word "asymptote" has to be considered here both on the sizes and the dynamical behaviours.

2.3 Transfer matrix

Let N^∞ be an arbitrary finite NSCA in $\mathbb{Z}^2$ of size n tending to infinity and order $3 \leq k \leq 6$. We denote its underlying interaction graph by $G^\infty = (V^\infty, E^\infty)$ and its associated Markov chain (whose related Markovian matrix is p^∞) by C^∞. In order to ease the analysis, let us give a new notation for configurations by using the set theory concept of cylinder. Indeed, in the sequel, a configuration $x \in \{0,1\}^n$ is denoted by $[A,B] \in \{0,1\}^n$ where $(A = \{i \in V^\infty \mid x_i = 1\}) \cap (B = \{i \in V^\infty \mid x_i = 0\}) = \emptyset$.

Now, consider the invariant measure μ of C^∞. By definition, μ satisfies the following projective and conditional relations. *Projective equations* are defined as:

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

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

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

where $\mu([\{i\},\emptyset])$ is the stationary probability for cell i to be at state 1 and $\Phi_i(A,B)$ is the conditional probability given in Equation 1 for cell i to be at state 1 at time step $t+1$ knowing configuration $[A,B]$ at time t such that $\mu(x_i(t+1) = 1 \mid [A,B]) = \Phi_i(A,B) = \mathsf{f} \circ \mathsf{g} \circ \mathsf{h}([A,B]) = \frac{e^{u_0 + \sum_{j \in \mathcal{N}_i^* \cap A} u_1 \cdot x_j(t) + \eta_i^k([A,B])}}{1 + e^{u_0 + \sum_{j \in \mathcal{N}_i^* \cap A} u_1 \cdot x_j(t) + \eta_i^k([A,B])}}$.

From now, we abuse the notation of η by considering that $\eta_i^k([A,B]) = \eta_i^k(A)$ for not weighing down the writing of equations. Furthermore, by hypothesis of the translation invariance property, N^∞ owns a spatial Markovian character that allows to study its dynamical behaviour by analysing only that of the sub-NSCA N whose interaction graph $G = (V,A)$ is the sub-graph of G^∞ restricted to vertices in the neighbourhood $\mathcal{N}_o$ of one arbitrary central cell o of N^∞[5]. Consider that the four cells 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 cells of $\mathcal{N}_o^*$, *i.e.*, $A,B \subseteq \mathcal{N}_o^*$, so that the non-linear term becomes:

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

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

Definition 2. *Let N^∞ be a finite* NSCA *of size n tending to infinity. Let N be the restriction of N^∞ 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 the μ's:*

[5]Notice that the choice of a central node is not mandatory in this theoretical framework but may have importance in the context of simulations because of the impossibility to simulate the dynamical behaviours of NSCAs whose size tends to infinity. In this case, focusing on a central cell 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 cells that are the less influenced by the boundary instances.

$$M = \left(\left(\begin{array}{c|cccc|cccccc|cccc|c}
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\
\Phi_4 & & \Phi_3 & & & & & \Phi_2 & & & & & \Phi_1 & & & \Phi_0
\end{array}\right)\right) \cdot \begin{pmatrix}
\mu([\{1,2,3,4\},\emptyset]) \\
\mu([\{2,3,4\},\{1\}]) \\
\mu([\{1,3,4\},\{2\}]) \\
\mu([\{1,2,4\},\{3\}]) \\
\mu([\{1,2,3\},\{4\}]) \\
\mu([\{3,4\},\{1,2\}]) \\
\mu([\{2,4\},\{1,3\}]) \\
\mu([\{2,3\},\{1,4\}]) \\
\mu([\{1,4\},\{2,3\}]) \\
\mu([\{1,3\},\{2,4\}]) \\
\mu([\{1,2\},\{3,4\}]) \\
\mu([\{4\},\{1,2,3\}]) \\
\mu([\{3\},\{1,2,4\}]) \\
\mu([\{2\},\{1,3,4\}]) \\
\mu([\{1\},\{2,3,4\}]) \\
\mu([\emptyset,\{1,2,3,4\}])
\end{pmatrix} = \begin{pmatrix}
\mu([\{2,3,4\},\emptyset]) \\
\mu([\{1,3,4\},\emptyset]) \\
\mu([\{1,2,4\},\emptyset]) \\
\mu([\{1,2,3\},\emptyset]) \\
\mu([\{3,4\},\{1\}]) \\
\mu([\{2,4\},\{1\}]) \\
\mu([\{2,3\},\{1\}]) \\
\mu([\{1,4\},\{2\}]) \\
\mu([\{1,3\},\{2\}]) \\
\mu([\{1,2\},\{3\}]) \\
\mu([\{4\},\{1,2\}]) \\
\mu([\{3\},\{1,2\}]) \\
\mu([\{2\},\{1,3\}]) \\
\mu([\{1\},\{2,3\}]) \\
\mu([\emptyset,\{1,2,3\}]) \\
\mu([\{o\},\emptyset])
\end{pmatrix},$$

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

3 Boundary sensitivity of attractive NSCAs

As evoked above, N^∞ is boundary sensitive if and only if two different instances of its covering system $\mathscr{S}$ admit distinct invariant measures. For the latter statement to hold, the structural parameters that characterise the system instances have to be intimately related [9, 17]. From a more local point of view, for N^∞ to be boundary sensitive, this invariant measure non-uniqueness needs to be retrieved at the level of the stationary probability of central cell o. Now, the transfer matrix M above characterises the asymptotic dynamical behaviour of o. From the lines above, it is easy to derive that a linear dependency between projective and conditional equations of the linear system of Definition 2 is necessary for o to behave asymptotically differently when subjected to two distinct instances of $\mathscr{S}$. So, *we are now going to prove a necessary and sufficient condition on* NSCA*s that validates the nullity of the determinant of their transfer matrices*.

In [3], Demongeot analysed some properties of Markov random fields and obtained a general formula characterising the nullity of the determinants of transfer matrices [3] such that 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* $\text{Det}M = 0 \iff \sum_{K\subseteq\mathscr{N}_o^*}(-1)^{|\mathscr{N}_o^*\setminus K|}\cdot\Phi_o(K,\mathscr{N}_o^*\setminus K) = 0$.

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 takes sense for NSCAs.

Definition 3. *Let N be an attractive* NSCA *of order k in $\mathbb{Z}^2$ and let i be an arbitrary cell of N. The non-linear term of i, denoted by η_i^k, is* symmetric *if and only if* $\forall K \subseteq \mathscr{N}_i^*,\ \eta_i^k(\mathscr{N}_i^*) = \eta_i^k(K) + \eta_i^k(\mathscr{N}_i^*\setminus K)$.

Let us prove that a particular case of the non-linear term symmetry is necessary and sufficient for Det$M =$ 0 to hold[6]. To do so, let us begin by studying properties of the general symmetric non-linear term. In

[6]The choice of this symmetry condition directly comes from the linear dependency of projective and conditional equations of the linear system of Definition 2 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 [5, 18] in the context of LSCAs, this peculiar relation is a counter-balancing relation between negative singleton potentials and positive couple potentials. From this

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 $-2\cdot u_0 - \sum_{j\in\mathcal{N}_o^*} u_1 - \eta_o^k(\mathcal{N}_o^* \setminus K)$. First, Lemma 2 gives a characterisation of the symmetric non-linear term.

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

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

Proof. Denoting $\eta_o^k(\mathcal{N}_o^*) - \eta_o^k(\mathcal{N}_o^* \setminus K) = \eta_{\text{sym}}$ and developing the left member of Equation 2 by definition of the non-linear term, trivially, we have $\forall K \subseteq \mathcal{N}_o^*$:

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

□

Now, let us express the symmetric property of the non-linear term by means of the conditional probabilities Φ_o's (the following lemma comes from [7] but its proof has been considerably simplified).

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

$$\forall K \subseteq \mathcal{N}_o^*,\ u_0 + \frac{\sum_{j\in\mathcal{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathcal{N}_o^*)}{2} = 0 \iff \Phi_o(K, \mathcal{N}_o^* \setminus K) + \Phi_o(\mathcal{N}_o^* \setminus K, K) = 1. \tag{3}$$

Proof. The proof is made directly by expanding and then simplifying the right member of Equation 3. First, we have:

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

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:

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

knowledge, it seemed natural that the same kind of counter-balancing relation occurs in NSCAs. Now, remark that the symmetry of the non-linear term constitutes a way to build non-linear interaction potentials of different parities of different signs in order to favour the counter-balancing effect.

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

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

and, by Lemma 2, we obtain:

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

□

In what follows, we use the same simplification for functions from $\{0,1\}^n$ to $\mathbb{R}^+$ as that used for η. Thus, given $[A,B] \in \{0,1\}^n$, a function $g([A,B])$ is denoted by $g(A)$.

Definition 4. *Let $g : \{0,1\}^n \to \mathbb{R}^+$ a function and V a set such that $|V| = n$. g is:*

- super-modular *if and only if* $\forall A, B \subseteq \{0,1\}^n,\ g(A \cup B) + g(A \cap B) \geq g(A) + g(B)$ *and*
- concave *if and only if* $\forall A, B \subseteq \{0,1\}^n, |A| \geq |B|,\ g(A) + g(V \setminus A) \leq g(B) + g(V \setminus B)$.

In [4, 15], the authors related the properties of attractivity and super-modularity with Proposition 1.

Proposition 1. *If a stochastic* CA *is attractive, then its local transition function is super-modular.*

From Definition 4, we deduce easily the following lemma.

Lemma 4. *Let N be an attractive* NSCA *of order k in $\mathbb{Z}^2$ and $G = (V,E)$ its interaction graph. If its local transition function Φ is super-modular and concave, then $\forall A \subseteq \{0,1\}^n,\ \Phi(V) + \Phi(\emptyset) = \Phi(A) + \Phi(V \setminus A)$.*

Now, from these intermediary results, we obtain the following theorem that gives a characterisation of the nullity of Det$M$ depending on the interaction potentials.

Theorem 1. *Let N be a finite attractive* NSCA *of size tending to infinity and order k in $\mathbb{Z}^2$. The following equation, that characterises a necessary condition of the boundary sensitivity of N, holds:*

$$\frac{\sum_{j \in \mathscr{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathscr{N}_o^*)}{2} = 0 \iff \mathrm{Det}M = 0. \tag{4}$$

Proof. ($\Longrightarrow$) From Lemma 1 and because of the parity of the cardinal of $\mathscr{N}_o^*$ (the number of subsets of Λ_o of even cardinal equals the number of subsets of Λ_o of odd cardinal), we have:

$$\begin{aligned} \mathrm{Det}M = 0 &\iff \sum_{K \subseteq \mathscr{N}_o^*} (-1)^{|\mathscr{N}_o^* \setminus K|} \cdot \Phi_o(K, \mathscr{N}_o^* \setminus K) = 0 \\ &\iff \sum_{K \subseteq \mathscr{N}_o^*} (-1)^{|\mathscr{N}_o^* \setminus K|} \times \frac{1}{2} \cdot (\Phi_o(K, \mathscr{N}_o^* \setminus K) + \Phi_o(\mathscr{N}_o^* \setminus K, K)) = 0. \end{aligned}$$

Then, from Lemma 3, we have:

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

Notice that the previous equation always holds under the general hypothesis of symmetry of the non-linear term of N (see Equation 3). As a result, following Lemmas 1, 2 and 3, we obtain $u_0 + \frac{\sum_{j \in \mathscr{N}_o^*} u_1}{2} + \frac{\eta_o^k(\mathscr{N}_o^*)}{2} = 0 \implies \mathrm{Det}M = 0$, which gives, by fixing the singleton potential u_0 to 0:

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

Thus, we obtain the expected sufficient condition of the nullity of Det$M$.

($\Longleftarrow$) First, notice that N is attractive by hypothesis. Consequently, following Proposition 1, the local transition function of its central cell o is super-modular. Moreover, remark that $\Phi_o = \mathsf{f} \circ \mathsf{g} \circ \mathsf{h}$ is a positive concave function. Indeed, $\forall x \in \{0,1\}^n$, $\Phi_o(x)$ is concave because, $\forall a \in \mathbb{R}^+$, so is the homographic function f. Hence, N verifies Lemma 4 whatever the parametric conditions in the u's, and we can write:

$$\forall K \subseteq \mathscr{N}_o^*,\ \mathrm{Det}M = 0 \implies \Phi_o(\mathscr{N}_o^*) + \Phi_o(\emptyset) \ = \ \Phi_o(K) + \Phi_o(\mathscr{N}_o^* \setminus K).$$

However, by definition of Φ_o, we have:

$$\forall K \subseteq \mathscr{N}_o^*,\ \Phi_o(\mathscr{N}_o^*) + \Phi_o(\emptyset) = \Phi_o(K) + \Phi_o(\mathscr{N}_o^* \setminus K)$$
$$\iff \ \frac{e^{u_0+a}}{1+e^{u_0+a}} + \frac{e^{u_0}}{1+e^{u_0}} = \frac{e^{u_0+a-b}}{1+e^{u_0+a-b}} + \frac{e^{u_0+b}}{1+e^{u_0+b}},$$

where a and b are positive functions of the interaction potentials u's. Because of the concavity of function Φ_o, such equalities hold if and only if $u_0 + a = u_0 = 0$. This results in:

$$\forall K \subseteq \mathscr{N}_o^*,\ \Phi_o(\mathscr{N}_o^*) + \Phi_o(\emptyset) \ = \ \Phi_o(K) + \Phi_o(\mathscr{N}_o^* \setminus K) \ = \ 1.$$

And, by Lemma 3, we conclude that:

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

and we obtain the expected necessary condition of the nullity of Det$M$. □

4 Conclusion

Throughout this paper, we have been interested in the issue of the boundary sensitivity of attractive NSCAs in $\mathbb{Z}^2$ of any non-linearity order and whose sizes tend to infinity. In particular, focusing on their asymptotic dynamical behaviours and defining their boundary sensitivity as their ability to converge towards different invariant measures, we have shown a necessary condition, entirely characterised by means of the interaction potentials defining such CA*s*, under which the latter become sensitive to fluctuations of instances of their boundary. Beyond the results presented, this work gives rise to many perspectives. Some of them, from a theoretical point of view only, are given below.

Of course, the question of the characterisation of the boundary sensitivity of NSCAs remains an open question and working in that direction seems pertinent. However, it is still an open question in the framework of LSCAs. Thus, the first step would be to deal with it before complexifying the problem by adding non-linearity. Another perspective concerns the nature of CAs addressed. Here, we have focused on attractive ones. Understanding how repulsive CAs behave when subjected to distinct boundary instances makes sense. The present knowledge on this subject tends to show that this issue is much more complicated. Indeed, no current mathematical methods have been emphasised to make this problem "tractable". To close the discussion on theoretical issues, let us list, without giving details on them, other points that seem all the more pertinent and interesting and that could thus be at the centre of further studies. These points deal with parametric constraints that have been made explicit here for the needs of the analysis but that could be relaxed, such as the underlying totality, translation invariance and synchronism properties. Remark that relaxing translation invariance would inevitably lead to a change of the underlying model of computation.

5 Acknowledgements

This work has been partially supported by the projects Synbiotic (ANR 2010 BLAN 0307 01) and Météding (RNSC AI10/11-L03908).

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