Math. Struct. in Comp. Science (2016), *vol.* 26, *pp.* 702–718. © Cambridge University Press 2014
doi:10.1017/S096012951400036X First published online 20 November 2014

Local cycles and dynamical properties of Boolean networks

PAUL RUET

CNRS, Laboratoire Preuves, Programmes et Systèmes, Université Paris Diderot - Paris 7, Case 7014, 75205 Paris Cedex 13, France
Email: ruet@pps.univ-paris-diderot.fr

Received 25 October 2011; revised 25 April 2014

We investigate the relationships between the dynamical properties of Boolean networks and properties of their Jacobian matrices, in particular the existence of local cycles in the associated interaction graphs. We define the notion of hereditarily bijective maps, and we use it to strengthen the property of unicity of a fixed point and to provide simplified proofs and generalizations of theorems relating attractors to the existence of local cycles, in particular local positive cycles. We then argue that this notion may not suffice to prove, under a suitable hypothesis such as the existence of a cyclic attractor or a stronger hypothesis, the existence of local negative cycles. We then consider a class of Boolean networks called and-or-nets, and for this class, we prove that the hypothesis of an antipodal attractive cycle implies the existence of a local negative cycle.

1. Introduction

Boolean networks represent the dynamic interaction of components which can take two values, 0 and 1. Introduced by von Neumann in the context of automata theory (von Neumann 1966), they have been extensively used to model genetic regulatory networks in particular, as well as other biological networks, since the early works of the biologists Kauffman (1969) and Thomas (1973). See also Kauffman (1993) for a more recent approach to these applications of Boolean networks.

The interest in Boolean networks has been recently renewed by:

i. the study of relationships between the dynamics and the structure of these networks along the line developed by Robert (1995), in particular the result of Shih and Dong (2005) relating fixed points to cycles in local interaction graphs;
ii. rules conjectured by Thomas and relating positive or negative cycles in the local interaction graphs to non-unicity of fixed points or sustained oscillation (Thomas 1981; Thomas and Kaufman 2001).

In Section 3, we define the notion of hereditarily bijective maps, and we show that hereditary bijectivity strengthens the property of unicity of a fixed point. This enables us to provide, in Section 5, simplified proofs and slight generalizations of theorems relating attractors to the existence of local cycles, in particular local positive cycles. We then argue in Section 6, that this notion may not suffice to prove, under a suitable hypothesis such as the existence of a cyclic attractor or under an even stronger hypothesis, the existence of

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

$$f_1(x) = (x_2 + 1)x_3$$
$$f_2(x) = (x_3 + 1)x_1$$
$$f_3(x) = (x_1 + 1)x_2$$

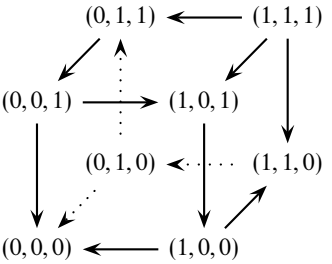


Fig. 1. A Boolean map $f : \mathbb{B}^3 \to \mathbb{B}^3$ and the asynchronous dynamics $\Gamma(f)$ associated to it. Consider for instance the point $x = (1, 0, 0)$ in $\Gamma(f)$: it has two outgoing edges to $x + e_1 = (0, 0, 0)$ and $x + e_2 = (1, 1, 0)$ because $f(x) = (0, 1, 0) = x + e_1 + e_2$.

local negative cycles. We then consider a class of Boolean networks, called and-or-nets and introduced in Richard and Ruet (2013), and for this class, we prove that the hypothesis of an antipodal attractive cycle implies the existence of a local negative cycle. Most of these results are bounded by explicit counterexamples.

2. Asynchronous Boolean networks

We need some preliminary definitions and notations. $\mathbb{B}$ denotes the set $\{0, 1\}$. Boolean sum $(+)$ and product $(\cdot)$ equip $\mathbb{B}$ with the structure of the field $\mathbb{F}_2$, while disjunction $(\alpha \vee \beta = \alpha + \beta + \alpha\beta)$ and product equip it with a tropical structure.

Let $\{e_1, \ldots, e_n\}$ be the canonical basis of the vector space $\mathbb{B}^n$, and for each $I \subseteq \{1, \ldots, n\}$, $e_I = \sum_{i \in I} e_i$. For $x, y \in \mathbb{B}^n$, $v(x, y)$ denotes the subset $I \subseteq \{1, \ldots, n\}$ such that $x + y = e_I$, and the Hamming distance $d(x, y)$ is defined as the cardinality of $v(x, y)$. Given $x \in \mathbb{B}^n$ and $I \subseteq \{1, \ldots, n\}$, the affine subspace $x[I]$ consists in all points y such that $y_i = x_i$ for each $i \notin I$; subspaces of the form $x[I]$ are called *subcubes* of $\mathbb{B}^n$. If $y = x + e_I$, the subcube $x[I]$ is also denoted by $[x, y]$.

Asynchronous Boolean networks can be equivalently presented in terms of directed graphs or in terms of Boolean maps. An *asynchronous Boolean network* can be defined:

— either as a directed graph whose vertex set is $\mathbb{B}^n$ and whose edges only relate vertices which are 1-distant from each other (for any edge from x to y, $d(x, y) = 1$);
— or as a map from $\mathbb{B}^n$ to $\mathbb{B}^n$.

The two presentations indeed carry the same information:

— Given a directed graph γ as above, we may define a map $\Phi(\gamma) : \mathbb{B}^n \to \mathbb{B}^n$ by $\Phi(\gamma)(x) = x + e_I$, where $\{(x, x + e_i), i \in I\}$ is the set of edges going from x in γ.
— Conversely, to a map $f : \mathbb{B}^n \to \mathbb{B}^n$ we may associate a directed graph $\Gamma(f)$ with vertex set $\mathbb{B}^n$ and an edge from x to y when for some i, $y = x + e_i$ and $f_i(x) \neq x_i$. In particular, if there is such an edge, $d(x, y) = 1$. We shall call $\Gamma(f)$ the *asynchronous dynamics* associated to f. Clearly, Γ and Φ are inverses of each other.

This definition is illustrated in Figure 1. As we shall consider asynchronous Boolean networks as dynamical systems, the coordinates i such that $f_i(x) \neq x_i$ may naturally be

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

considered as the *degrees of freedom* of x, and it is worth observing that asynchronous Boolean networks are nondeterministic, in the sense that, in general, points have several degrees of freedom. Note that the number of degrees of freedom of x is the out-degree of x in $\Gamma(f)$.

A word should be said here about the reason for considering such asynchronous Boolean dynamics in this paper, rather than, e.g. the iteration of a map from $\mathbb{B}^n$ to itself (which we might call a synchronous dynamics). A motivation arises from applications to genetic networks, in which n genes interact through (activatory and inhibitory) regulatory processes. Such a dynamical system, whose states are n-tuples of concentrations in regulatory products, is governed by differential equations with very strong threshold effects (sigmoids), which are often conveniently approximated by piecewise-linear equations. These piecewise-linear equations may in turn be discretized: an $x \in \mathbb{B}^n$ then represents a tuple of discretized concentrations, where, in case each gene has a unique threshold, $x_i = 1$ when the concentration in the regulatory product i is above a threshold, 0 otherwise. Through this discretization, all points in a region of $\mathbb{R}^n_+$ delimited by the n hyperplanes defined by thresholds are mapped to the same $x \in \mathbb{B}^n$. Call this region the region of x. Now, the choice of focussing on the asynchronous dynamics (where a unique regulatory product i is updated at a time) follows from the fact that trajectories in the original differential or piecewise-linear equation almost surely (in the sense of measure theory) cross one threshold hyperplane at a time. The successors of x in $\Gamma(f)$ correspond to the hyperplanes crossed by trajectories starting in the region of x.

2.1. *Dynamics*

Let $f : \mathbb{B}^n \to \mathbb{B}^n$. A *trajectory* is a path in $\Gamma(f)$. An *attractor* is a terminal strongly connected component of $\Gamma(f)$. An attractor which is not a singleton (i.e. which does not consist in a fixed point) is called a *cyclic attractor*. Since $\Gamma(f)$ must have some attractor, it has a cyclic attractor if f has no fixed point. *Attractive cycles*, i.e. cyclic trajectories θ such that for each point $x \in \theta$, $d(x, f(x)) = 1$, are examples of cyclic attractors. Observe that attractive cycles are deterministic, since any point in θ has a unique degree of freedom.

Definition (first return). Given an attractive cycle θ and points x, y on θ, the set of points on the trajectory from x to y in θ, x and y excluded, is denoted by $\theta(x, y)$. If $x \neq y$, $f(x) + x = f(y) + y$ and for any $z \in \theta(x, y)$, $f(x) + x \neq f(z) + z$, y is called the *first return of* x.

Observe that, by definition of an attractive cycle θ, for each point x on θ, there exist an odd number of points y on θ such that $y \neq x$ and $f(x) + x = f(y) + y$, hence at least one. A special class of attractive cycles, called antipodal attractive cycles and defined below, will be considered in Section 6.2.

Definition (antipodal attractive cycle). An attractive cycle θ is said to be *antipodal* when θ is of the form $\{x^0, x^1, \ldots, x^{k-1}, y^0, y^1, \ldots, y^{k-1}\}$ and for any $i \in \{0, \ldots, k-1\}$, y^i is the first return of x^i.

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

f has a cyclic attractor if and only if it is not *weakly terminating* (i.e. for some $x \in \mathbb{B}^n$, all trajectories leaving x are infinite). A stronger form of weak termination may be defined as follows.

Definition (direct trajectories and termination). Given $f : \mathbb{B}^n \to \mathbb{B}^n$, a path from $x \in \mathbb{B}^n$ to $y \in \mathbb{B}^n$ in $\Gamma(f)$ is called a *direct trajectory* when its length is minimal, i.e. equals $d(x, y)$. And $\Gamma(f)$ is said to be *directly terminating* when for any point $x \in \mathbb{B}^n$ there exists a direct trajectory from x to some fixed point.

For any subcube κ, let $\pi_\kappa : \mathbb{B}^n \to \kappa$ be the projection onto κ, defined as follows: if $\kappa = x[I]$,

$$(\pi_\kappa(y))_i = \begin{cases} y_i & \text{if } i \in I \\ x_i & \text{otherwise.} \end{cases}$$

Let also $\iota_\kappa : \kappa \to \mathbb{B}^n$ be the inclusion map. It is then immediate that $\pi_\kappa \circ \iota_\kappa$ is the identity. For any $f : \mathbb{B}^n \to \mathbb{B}^n$, let

$$f\restriction_\kappa = \pi_\kappa \circ f \circ \iota_\kappa : \kappa \to \kappa.$$

The asynchronous dynamics $\Gamma(f\restriction_\kappa)$ is easily shown to be the subgraph of $\Gamma(f)$ induced by vertices in κ, a characterization which may be taken as an alternative, more intuitive, definition of $f\restriction_\kappa$.

Lemma 2.1. If f has at least two attractors, then for some subcube κ, $f\restriction_\kappa$ has at least two fixed points.

Proof. Indeed, let A and B be any two attractors of $\Gamma(f)$ and $(a, b) \in A \times B$ be any pair such that $d(a, b)$ is minimal: then a and b are fixed points of $f\restriction_{[a,b]}$. □

2.2. *Translations*

The group $\mathbb{B}^n$ acts on the set of maps from $\mathbb{B}^n$ to itself by translation: if $x \in \mathbb{B}^n$ and $f : \mathbb{B}^n \to \mathbb{B}^n$, $f + x$ is the map $y \mapsto f(y) + x$. Since $\mathrm{d}(f + x) = \mathrm{d}f$, the orbits under translation are exactly the equivalence classes of maps for the equivalence relation given by: $f \sim g$ if and only if $\mathrm{d}f = \mathrm{d}g$.

Lemma 2.2.

i. If $f + \mathrm{id}$ is bijective, then f has a unique fixed point.
ii. Under the action by translation, an orbit of maps from $\mathbb{B}^n$ to itself contains a map with no fixed point if and only if it contains a map with at least two fixed points.

Proof. The first claim is immediate, as $f + \mathrm{id}$ takes the value 0 exactly once.

For the second claim, it suffices to observe that if f has no fixed point, $f + \mathrm{id}$ is a non-bijective map from a finite set to itself, hence it is not injective: therefore, for some z, there exist distinct points x, y such that $(f + \mathrm{id})(x) = (f + \mathrm{id})(y) = z$ and $f + z$ has two fixed points. On the other hand, if f has two fixed points, $f + \mathrm{id}$ is not bijective, hence not surjective and does not take some value z: then $f + z$ has no fixed point. □

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

Lemma 2.3. The set of maps $f : \mathbb{B}^n \to \mathbb{B}^n$ such that for each subcube κ, $f\restriction_\kappa$ has a unique fixed point, is closed under translation.

Proof. Let F_n be the set of maps $f : \mathbb{B}^n \to \mathbb{B}^n$ such that for each subcube κ, $f\restriction_\kappa$ has a unique fixed point. Since the group of translations is generated by translations by basis vectors e_i, to prove the lemma, it suffices to prove, by induction on n, that for any $f \in F_n$ and $i \in \{1, \ldots, n\}$, $f + e_i \in F_n$.

— For $n = 1$, the maps with a unique fixed point are the constant maps, and constant maps are closed under translation.

— If $n > 1$, let $f \in F_n$, $i \in \{1, \ldots, n\}$ and $g = f + e_i$. Let κ_0 and κ_1 be the $(n-1)$-dimensional subcubes defined respectively by $x_i = 0$ and $x_i = 1$. By induction hypothesis, $g\restriction_{\kappa_0}$ has a unique fixed point x and $g\restriction_{\kappa_1}$ has a unique fixed point y. On the other hand, since $\mathbb{B}^n = \kappa_0 \cup \kappa_1$, f has a unique fixed point, which needs to be either x or y, say it is x. Then $f(y) = y + e_i$ and $g(y) = y$. Moreover, $f(x) = x$, hence $g(x) \neq x$, and we may conclude that y is the unique fixed point of g, hence that $g \in F_n$.

□

However, it is worth observing that the set of maps which have a unique fixed point is not closed under translation: the map $f : \mathbb{B}^2 \to \mathbb{B}^2$ given by $f(x) = (x_1x_2 + x_2 + 1, x_1x_2 + x_2 + 1)$ has a unique fixed point $(1, 1)$, but $f + e_1$ has no fixed point and $f + e_2$ has 2 fixed points.

3. Hereditarily bijective maps

In Section 5, we shall prove in particular that the theorem of Shih and Dong (2005) on the existence and unicity of fixed points can be reviewed in terms of hereditarily bijective maps.

Definition (hereditarily bijective and hereditarily ufp maps). A map $f : \mathbb{B}^n \to \mathbb{B}^n$ is called *hereditarily bijective* (resp. *hereditarily ufp*) when for any subcube κ, $f\restriction_\kappa$ is bijective (resp. has a unique fixed point).

Hereditarily bijective maps may be intuitively characterized as follows. Call a pair $(x, y) \in \mathbb{B}^n \times \mathbb{B}^n$ a *mirror pair* of $f : \mathbb{B}^n \to \mathbb{B}^n$ when $(f + \mathrm{id})\restriction_{[x,y]}(x) = (f + \mathrm{id})\restriction_{[x,y]}(y)$, i.e. when x and y have the same degrees of freedom for the projected map $f\restriction_{[x,y]}$.

Proposition 3.1. For any $f : \mathbb{B}^n \to \mathbb{B}^n$, $f + \mathrm{id}$ is hereditarily bijective if and only if f has no mirror pair.

Proof. If f has a mirror pair (x, y), then $(f + \mathrm{id})\restriction_{[x,y]}$ is clearly not bijective and $f + \mathrm{id}$ is not hereditarily bijective.

Conversely, if $f + \mathrm{id}$ is not hereditarily bijective, $(f + \mathrm{id})\restriction_\kappa(x) = (f + \mathrm{id})\restriction_\kappa(y)$ for some subcube κ and $x, y \in \kappa$, hence $(f + \mathrm{id})\restriction_{[x,y]}(x) = (f + \mathrm{id})\restriction_{[x,y]}(y)$ and (x, y) is a mirror pair of f. □

Theorem 3.1. For any $f : \mathbb{B}^n \to \mathbb{B}^n$, $f + \mathrm{id}$ is hereditarily bijective if and only if f is hereditarily ufp.

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

Proof. If for each subcube κ, $(f+\mathrm{id})\restriction_\kappa$ is bijective, the fact that all the $f\restriction_\kappa$ have a unique fixed point follows from Lemma 2.2.

On the other hand, in order to prove that for any $n \geqslant 1$ and any $f : \mathbb{B}^n \to \mathbb{B}^n$, if f is hereditarily ufp, then $f+\mathrm{id}$ is hereditarily bijective, it suffices to prove that for any n and f, if $f\restriction_\kappa$ has a unique fixed point for each subcube κ, then $f+\mathrm{id}$ is bijective: this is because the hypothesis is closed under restriction. Assume this is wrong, so that there exists some $f : \mathbb{B}^n \to \mathbb{B}^n$ such that $f+\mathrm{id}$ is not bijective while $f\restriction_\kappa$ has a unique fixed point for each subcube κ. Since $f+\mathrm{id}$ is not bijective, the preimage $(f+\mathrm{id})^{-1}(z)$ of some z is not a singleton, hence $(f+z+\mathrm{id})^{-1}(0)$ is not a singleton and $f+z$ does not have a unique fixed point. But by Lemma 2.3, this contradicts the hypothesis on f, because f and $f+z$ are in the same orbit under translation. □

Corollary 3.1. If $f+\mathrm{id}$ is hereditarily bijective, then $\Gamma(f)$ has a unique attractor, this attractor is a fixed point and $\Gamma(f)$ is directly terminating (in particular, it is weakly terminating).

Proof. Under the hypothesis of the Corollary, by Theorem 3.1, for each subcube κ, $f\restriction_\kappa$ has a unique fixed point. Lemma 2.1 then ensures that this fixed point is the only attractor of $\Gamma(f)$. Let now x be the unique fixed point of f and let Y be the set of points $y \in \mathbb{B}^n$ such that $\Gamma(f)$ has no direct trajectory from y to x. Assume for a contradiction that $\Gamma(f)$ is not directly terminating. This implies $Y \neq \emptyset$ and we may choose $y \in Y$ such that $d(x,y)$ is minimal: then x and y are fixed points for $f\restriction_{[x,y]}$, and since $y \neq x$, it follows from Lemma 2.2 that $(f+\mathrm{id})\restriction_{[x,y]}$ is not bijective. □

The converse is obviously wrong, i.e. direct termination does not imply hereditary bijectivity: $f(x_1,x_2) = (0, x_1x_2)$ is a counterexample. Moreover, under the hypothesis of the corollary, $\Gamma(f)$ need not to be strongly terminating, i.e. Noetherian: the map $f : \mathbb{B}^3 \to \mathbb{B}^3$ defined in Figure 1 is such that $f+\mathrm{id}$ is hereditarily bijective, but $\Gamma(f)$ has a (non-attractive) cycle $(1,0,0) \to (1,1,0) \to (0,1,0) \to (0,1,1) \to (0,0,1) \to (1,0,1) \to (1,0,0)$.

On the other hand, the fact $f+\mathrm{id}$ is bijective (a weaker hypothesis) does not suffice to conclude that $\Gamma(f)$ is directly terminating, not even weakly terminating: for instance, $f : \mathbb{B}^2 \to \mathbb{B}^2$ defined by $f(x_1,x_2) = (x_1+x_2, x_1+x_2)$ has a cyclic attractor $\{(1,1),(1,0),(0,1)\}$.

Since $\Gamma(f)$ must have some attractor, it has at least one fixed point or a cyclic attractor, and the following is an immediate consequence of the above corollary.

Corollary 3.2. If f has no fixed point or $\Gamma(f)$ has a cyclic attractor, then $f+\mathrm{id}$ is not hereditarily bijective.

4. Derivatives of Boolean maps

4.1. *Preliminaries on Boolean matrices*

The determinant $\det(M)$ of an $n \times n$ matrix M with entries in $\mathbb{B}$, which may be defined by $\det(M) = \sum_{\sigma \in \mathfrak{S}_n} \prod_{i=1}^n M_{\sigma(i),i}$, satisfies the usual properties of commutation with product (the product of matrices being defined with $+$ and $\cdot$) and characterization of invertibility: M is invertible if and only if $\det(M) = 1$. The identity matrix is denoted by $\mathscr{I}$.

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

If N is an nilpotent matrix, then $\mathscr{I}+N$ is invertible, with inverse $\sum_{i\geqslant 0} N^i$. The converse is obviously wrong because for instance, both M and $\mathscr{I}+M$ may be invertible, already in dimension 2.

The graph *associated* to the $n \times n$ matrix M with entries in $\mathbb{B}$ is the simple directed graph with vertex set $\{1,\dots,n\}$ whose adjacency matrix is the transpose of M : it has an edge from i to j if and only if $M_{j,i} = 1$. Recall that a cycle in a graph is a non-empty subgraph of the form $k_1 \to k_2 \to \cdots \to k_p \to k_1$ such that $k_1,\dots,k_p$ are all different: the cycles we shall consider are all elementary. Recall also that a loop is a cycle such that $p = 1$.

All the graphs considered in the article are directed and simple.

Lemma 4.1. If the graph associated to M has no cycle, then M is nilpotent.

Proof. For any $k > 0$, the graph G_k associated to M^k has an edge from i to j if and only if the number of paths of length k from i to j in G_1 is odd, hence G_k has no cycle. Let I_k be the set of vertices of G_k which are not the target of any edge. For each $i \in I_k$, the i^{th} row of M^k is zero, and by hypothesis, $I_1 \neq \varnothing$. In case $M^k \neq 0$, the acyclic graph G_k has a vertex $i \notin I_k$, whose incoming edges all have their source in I_k. Then, the set of zero rows in M^{k+1} is larger, i.e. I_k is a strict subset of I_{k+1}. This proves that $I_n = \{1,\dots,n\}$, i.e. $M^n = 0$. □

The converse is wrong: the 2×2 matrix whose four entries all equal 1 is nilpotent of order 2, while its associated graph has three cycles.

4.2. *Derivatives*

The definition of the discrete derivative of Boolean maps has been introduced in several occasions (Kim 1982; Rudeanu 1974) and developed in Robert (1995).

Given $\varphi : \mathbb{B}^n \to \mathbb{B}$ and $i \in \{1,\dots,n\}$, the *discrete ith partial derivative* $\partial\varphi/\partial x_i = \partial_i\varphi : \mathbb{B}^n \to \mathbb{B}$ maps each $x \in \mathbb{B}^n$ to

$$\partial_i\varphi(x) = \varphi(x) + \varphi(x + e_i).$$

Higher order derivatives $\partial^k\varphi/\partial x_{i_1}\cdots\partial x_{i_k} = \partial_I\varphi : \mathbb{B}^n \to \mathbb{B}$ can be defined, for each $I = \{i_1,\dots,i_k\} \subseteq \{1,\dots,n\}$, by

$$\partial_I\varphi(x) = \sum_{J\subseteq I} \varphi(x + e_J),$$

in such a way that $\partial_\varnothing\varphi = \varphi$, $\partial_i = \partial_{\{i\}}$ and

$$\partial_I\partial_J = \partial_J\partial_I = \begin{cases} \partial_{I\cup J} & \text{if } I \cap J = \varnothing \\ 0 & \text{otherwise.} \end{cases}$$

The second case follows from the observation that $\partial_i\partial_i = 0$. For a map $f : \mathbb{B}^n \to \mathbb{B}^m$, its derivative $\mathrm{d}f$ maps each $x \in \mathbb{B}^n$ to the *discrete Jacobian matrix* $\mathscr{J}(f)(x)$, which is the $m \times n$ matrix with entries $\mathscr{J}(f)(x)_{i,j} = \partial_j f_i(x)$.

It is immediate that the operator d is linear: $\mathrm{d}(f+g) = \mathrm{d}f + \mathrm{d}g$ for parallel maps $f, g : \mathbb{B}^n \to \mathbb{B}^m$. However, d is not functorial, contradicting a claim of Bazsó (2000): for

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

a simple counterexample to the chain rule, take $f : \mathbb{B}^2 \to \mathbb{B}^2$ to be the map $f(x_1, x_2) = (x_1, x_1x_2)$ and $g : \mathbb{B}^2 \to \mathbb{B}$ to be the product; then $g \circ f = g$ and

$$\mathscr{J}(f)(x) = \begin{pmatrix} 1 & 0 \\ x_2 & x_1 \end{pmatrix}$$

$$\mathscr{J}(g)(f(x)) = (x_1x_2, x_1)$$

so that $\mathscr{J}(g)(f(x)) \cdot \mathscr{J}(f)(x) = (0, x_1)$, while $\mathscr{J}(g \circ f)(x) = \mathscr{J}(g)(x) = (x_2, x_1)$. A simple computation shows that the chain rule holds in case g is affine, i.e. when $\mathscr{J}(g)(x)$ is independent of x.

Discrete derivatives satisfy the Taylor formula

$$\varphi(x + y) = \sum_{I \subseteq v(x,y)} \partial_I \varphi(x)$$

and a variant of Leibniz rule

$$\partial_i(\varphi\psi) + \partial_i\varphi\partial_i\psi = \varphi\partial_i\psi + \psi\partial_i\varphi.$$

The following local inverse theorem holds: if $f : \mathbb{B}^n \to \mathbb{B}^n$ and $x \in \mathbb{B}^n$ are such that $\mathscr{J}(f)(x)$ is invertible, then the restriction of f to the unit ball $B(x, 1)$, defined by $d(x, y) \leqslant 1$, is injective. This is simply because if $f(x) = f(x + e_i)$, the i^{th} column $\partial_i f(x)$ of $\mathscr{J}(f)(x)$ is 0, and if $f(x + e_i) = f(x + e_j)$, $\partial_i f(x) = \partial_j f(x)$ and $\mathscr{J}(f)(x)$ has two identical columns. But since f is only locally injective and need not restrict to a bijection from $B(x, 1)$ to $B(f(x), 1)$, no simple implicit function theorem holds.

5. Dynamics and structure

5.1. *Cycles*

A *signed directed graph* is a directed graph with a sign, + or −, attached to each edge, and the *sign* of a cycle is defined to be the product of the signs of its edges.

Given $f : \mathbb{B}^n \to \mathbb{B}^n$ and $x \in \mathbb{B}^n$, recall from Remy *et al.* (2008) that $\mathscr{G}(f)(x)$, the *interaction graph of f at x*, is defined to be the signed directed graph with vertex set $\{1, \ldots, n\}$ and with an edge from j to i when $\mathscr{J}(f)(x)_{i,j} = 1$, with positive sign when

$$x_j = f_i(x),$$

and negative sign otherwise. In particular, the transpose of $\mathscr{J}(f)(x)$ is the adjacency matrix of the graph underlying $\mathscr{G}(f)(x)$.

The following equivalent definition of $\mathscr{G}(f)(x)$ gives the intuition for the positive and negative signs of edges: $\mathscr{G}(f)(x)$ is the signed directed graph with vertex set $\{1, \ldots, n\}$ and with an positive (resp. negative) edge from j to i when the following map from $\mathbb{B}$ to itself:

$$\alpha \mapsto f_i(x_0, \ldots, x_{j-1}, \alpha, x_{j+1}, \ldots, x_n)$$

is the identity (resp. the negation), i.e. when it is strictly increasing (resp. decreasing).

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

The signed directed graph $\mathscr{G}(f)$ has vertex set $\{1,\dots,n\}$ and a positive (resp. negative) edge from i to j when for some $x \in \mathbb{B}^n$, $\mathscr{G}(f)(x)$ has a positive (resp. negative) edge from i to j. For all $x \in \mathbb{B}^n$, $\mathscr{G}(f)(x)$ is therefore a subgraph of $\mathscr{G}(f)$. In particular, a cycle in $\mathscr{G}(f)(x)$ for some x is called a *local* cycle of $\mathscr{G}(f)$.

The following lemma was proved in Remy and Ruet (2007).

Lemma 5.1. If $f : \mathbb{B}^n \to \mathbb{B}^n$, $\kappa = x[I]$ is a subcube and $y \in \kappa$, then $\mathscr{G}(f\restriction_\kappa)(y)$ is the induced subgraph of $\mathscr{G}(f)(\iota_\kappa(y))$ with vertex set I. (Here, we identify κ with $\{0,1\}^I$ and $f\restriction_\kappa$ with a map from $\{0,1\}^I$ to itself.)

Theorem 5.1. Let $f : \mathbb{B}^n \to \mathbb{B}^n$. If $f + \mathrm{id}$ is not bijective, then there exist two different points $x, y \in \mathbb{B}^n$ such that $\mathscr{G}(f)(x)$ and $\mathscr{G}(f)(y)$ have a cycle.

Proof. To prove this theorem, first observe that as a non-bijective map from a finite set to itself, $f + \mathrm{id}$ is not injective: some point $z \in \mathbb{B}^n$ has a preimage of cardinality at least 2 under $f + \mathrm{id}$. Consider the partially ordered set E_z of subcubes κ, ordered by inclusion, such that $\pi_\kappa(z)$ has a preimage of cardinality at least 2 under $(f + \mathrm{id})\restriction_\kappa$. By hypothesis, $E_z \neq \emptyset$. Let κ be a minimal subcube of E_z, and let $x, y \in \kappa$ be distinct points mapped by $(f + \mathrm{id})\restriction_\kappa$ to $z\restriction_\kappa$. Since κ is minimal in E_z, x and y are antipodes in κ, i.e. $\kappa = [x, y]$. Recall that $v(x, y)$ denotes the subset $I \subseteq \{1,\dots,n\}$ such that $x + y = e_I$.

— If $v(x,y)$ is a singleton $\{i\}$, then $y = x + e_i$ and $(f + \mathrm{id})_i(x) = (f + \mathrm{id})_i(y)$, as a consequence $\partial_i f_i(x) = f_i(x) + f_i(x + e_i) = \partial_i f_i(x + e_i) = 1$, hence $\mathscr{G}(f)(x)$ and $\mathscr{G}(f)(y)$ have an edge from i to itself.

— If on the other hand $d(x, y) \geqslant 2$, for any $i \in v(x, y)$, let λ_i be the subcube $[x+e_i, y]$, which is smaller than κ: then $(f + \mathrm{id})\restriction_{\lambda_i}(x + e_i) \neq \pi_{\lambda_i}(z)$, since otherwise λ_i would have two different points $x+e_i$ and y mapped by $(f+\mathrm{id})\restriction_{\lambda_i}$ to $\pi_{\lambda_i}(z)$, and λ_i would belong to E_z, contradicting minimality. Therefore, for any $i \in v(x, y)$, $(f+\mathrm{id})\restriction_{\lambda_i}(x+e_i) \neq (f+\mathrm{id})\restriction_{\lambda_i}(x)$, hence there exists $j \in v(x, y)$, such that $j \neq i$ and $\partial_i f_j(x) = f_j(x) + f_j(x + e_i) = 1$, and $\mathscr{G}(f)(x)$ has an edge from i to j. As a consequence, $\mathscr{G}(f)(x)$ has an infinite path, hence a cycle, and by symmetry, so has $\mathscr{G}(f)(y)$.

□

An alternative proof may be obtained by considering the set of subcubes κ such that $(f + \mathrm{id})\restriction_\kappa$ is not bijective.

Theorem 5.1 provides alternative proofs of the following generalizations of results from Shih and Dong (2005), Remy *et al.* (2008) and Richard (2010).

Corollary 5.1. If $\Gamma(f)$ has a cyclic attractor (in particular if f has no fixed point, or has an attractive cycle) or has at least two attractors, then there exist two different points $x, y \in \mathbb{B}^n$ such that $\mathscr{G}(f)(x)$ and $\mathscr{G}(f)(y)$ have a cycle.

Proof. If $\Gamma(f)$ has several attractors or has a cyclic attractor (i.e. is not weakly terminating), then for some subcube κ, $(f + \mathrm{id})\restriction_\kappa$ is not bijective, according to Corollary 3.1. Then the conclusion follows from Theorem 5.1 and Lemma 5.1. □

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

Corollary 5.2. If $\mathscr{G}(f)$ has no local cycle, then $f + \mathrm{id}$ is hereditarily bijective.

Corollary 5.3. If $\mathscr{G}(f)$ has no local cycle, then f is hereditarily ufp, in particular f has a unique fixed point.

It is worth mentioning that the converse to, e.g., Corollary 5.2, does not hold: for the map $f : \mathbb{B}^3 \to \mathbb{B}^3$ defined by $f(x) = ((x_2 + 1)x_3, (x_3 + 1)x_1, (x_1 + 1)x_2)$, already considered in Section 3, $\mathscr{G}(f)(0)$ has a cycle, while $f + \mathrm{id}$ is hereditarily bijective.

5.2. *Positive cycles*

Lemma 5.2. Let $f : \mathbb{B}^n \to \mathbb{B}^n$ and $x \in \mathbb{B}^n$. If C is a cycle of $\mathscr{G}(f)(x)$ with vertex set I, then C is positive (resp. negative) when x has an even (resp. odd) out-degree in $\Gamma(f)$, i.e. when $\sum_{i\in I}(x_i + f_i(x)) = 0$ (resp. 1). In particular, if x is a fixed point of f and C is any cycle in $\mathscr{G}(f)(x)$, then C is positive.

Proof. The first assertion follows from the fact that $C = k_1 \to \cdots \to k_p \to k_1 = k_{p+1}$ is positive if and only if

$$\sum_{i=1}^{p}(x_{k_i} + f_{k_i+1}(x)) = 0 = \sum_{i=1}^{p} x_{k_i} + \sum_{i=1}^{p} f_{k_i}(x) = \sum_{i=1}^{p}(x_{k_i} + f_{k_i}(x)). \qquad \square$$

The above results induce a slight generalization of a result from Remy *et al.* (2008) and Richard (2010).

Corollary 5.4. If $f : \mathbb{B}^n \to \mathbb{B}^n$ has at least two attractors, then there exist two different points $x, y \in \mathbb{B}^n$ such that $\mathscr{G}(f)(x)$ and $\mathscr{G}(f)(y)$ have a positive cycle.

Proof. By Lemma 2.1, some projection $f\restriction_\kappa$ has two fixed points. Hence $f\restriction_\kappa + \mathrm{id}$ is not bijective, and by Theorem 5.1 applied to $f\restriction_\kappa$, there exist two points x, y such that $\mathscr{G}(f\restriction_\kappa)(x)$ and $\mathscr{G}(f\restriction_\kappa)(y)$ have cycles. These cycles are also cycles of $\mathscr{G}(f)(x)$ and $\mathscr{G}(f)(y)$ by Lemma 5.1, and are positive by Lemma 5.2. $\square$

6. Negative cycles

6.1. *Hereditary bijectivity again*

Theorem 3.1, and the above results on the existence of cycles and positive cycles, suggest to look for a proof of existence of local negative cycles in $\mathscr{G}(f)$ through (hereditary) bijectivity of $f + \mathrm{id}$. The following lemma strengthens this possibility.

Lemma 6.1. If $f + \mathrm{id}$ is bijective, then $\mathscr{G}(f)$ has a local positive loop if and only if it has a local negative loop.

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

Proof. Recall that a loop is a cycle of length 1. The number of directed edges in $\Gamma(f)$ equals

$$\begin{aligned}
&\sum_{x\in\mathbb{B}^n} \text{cardinality}\big(\{i \text{ such that } f_i(x)\neq x_i\}\big)\\
&\quad= \sum_{x\in\mathbb{B}^n} d(f(x)+x,0)\\
&\quad= \sum_{x\in\mathbb{B}^n} d(x,0) \qquad \text{because } f+\mathrm{id} \text{ is bijective}\\
&\quad= n\cdot 2^{n-1},
\end{aligned}$$

which is also the number of (non-directed) edges of the cube $\mathbb{B}^n$. Therefore, if $\mathscr{G}(f)$ has a local positive loop, then some edge of $\mathbb{B}^n$ carries no orientation in $\Gamma(f)$; by the above equality, some (other) edge of $\mathbb{B}^n$ has to carry both orientations in $\Gamma(f)$, and $\mathscr{G}(f)$ has a local negative loop. The converse implications hold for the same reason. □

However, it is not true that if $f+\mathrm{id}$ is bijective, even hereditarily bijective, then $\mathscr{G}(f)$ has a local positive cycle if and only if it has a local negative cycle. For a counterexample, let $f:\mathbb{B}^4\to\mathbb{B}^4$ be defined by

$$\begin{aligned}
f_1(x) &= x_4(x_2+1)(x_3+1)\\
f_2(x) &= x_1(x_3+1)(x_4+1)\\
f_3(x) &= x_2(x_4+1)(x_1+1)\\
f_4(x) &= x_3(x_1+1)(x_2+1);
\end{aligned}$$

it is a straightforward computation to check that $f+\mathrm{id}$ is hereditarily bijective, but

$$\mathscr{J}(f)(x) = \begin{pmatrix}
0 & x_4(x_3+1) & x_4(x_2+1) & (x_2+1)(x_3+1)\\
(x_3+1)(x_4+1) & 0 & x_1(x_4+1) & x_1(x_3+1)\\
x_2(x_4+1) & (x_4+1)(x_1+1) & 0 & x_2(x_1+1)\\
x_3(x_2+1) & x_3(x_1+1) & (x_1+1)(x_2+1) & 0
\end{pmatrix}$$

and the only local cycle is the positive cycle $1\to 2\to 3\to 4\to 1$ of $\mathscr{G}(f)(0)$.

On the other hand, the following lemma suggests to use the invertibility of some Jacobian matrix $\mathscr{J}(f)(x)$ to exhibit a negative cycle.

Lemma 6.2. If $x\in\mathbb{B}^n$ has an odd out-degree in $\Gamma(f)$ (i.e. $\sum_{i=1}^n x_i+f_i(x)=1$) and $\mathscr{J}(f)(x)$ is invertible, then $\mathscr{G}(f)$ has a local negative cycle.

Proof. $\mathscr{J}(f)(x)$ is invertible if and only if

$$\det \mathscr{J}(f)(x) = 1 = \sum_{\sigma\in\mathfrak{S}_n}\prod_{i=1}^n \mathscr{J}(f)(x)_{\sigma(i),i},$$

therefore $\prod_{i=1}^n \mathscr{J}(f)(x)_{\sigma(i),i}=1$ for at least one permutation $\sigma\in\mathfrak{S}_n$ (actually an odd number of permutations). Furthermore, σ is a product of disjoint cycles $C_1,\dots,C_k$, and the assumption $\sum_{i=1}^n(x_i+f_i(x))=1$ implies that at least one (actually an odd number) of these cycles is negative. □

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

But Appendix A shows that the invertibility of the Jacobian matrices $\mathscr{J}(f)(x)$ is not related to the bijectivity of f in a simple way, and it is easy to convince oneself that it is not related to the bijectivity of $f + \mathrm{id}$ either.

It is therefore unclear whether hereditary bijectivity can turn out to be useful, in general, for the question of the existence of local negative cycles (under some hypothesis on the dynamics).

The difficulty of this question is emphasized by the following theorem, which establishes that negative cycles, if any, may be localized only away from the cyclic attractor.

Theorem 6.1. The fact that $f : \mathbb{B}^n \to \mathbb{B}^n$ has an attractive cycle C does not imply that for some $x \in C$, $\mathscr{G}(f)(x)$ has a negative cycle.

Proof. Let $n \geqslant 4$ and define $f : \mathbb{B}^n \to \mathbb{B}^n$ by its asynchronous dynamics $\Gamma(f)$, which consists in:

— the $2n$ edges of the antipodal attractive cycle

$$x^0 \to x^1 \to \cdots \to x^{n-1} \to y^0 \to y^1 \to \cdots \to y^{n-1} \to x^0,$$

where $x^i = e_{\{1,\ldots,i\}}$ and $y^i = x^i + e_{\{1,\ldots,n\}}$,

— the $2n-4$ edges

$$x^i + e_{i-1} \to x^i \text{ and } y^i + e_{i-1} \to y^i$$

for $i \in \{2,\ldots,n-1\}$, and the 4 edges

$$e_{n-1} \to x^0 = 0,\ x^1 + e_n \to x^1,\ y^0 + e_{n-1} \to y^0,\ y^1 + e_n \to y^1.$$

Then, the above antipodal attractive cycle C is the unique cyclic attractor of f. Furthermore, in $\mathscr{G}(f)(0)$, the only edge with source 1 is the edge $1 \to 2$ and there is no edge with source 2 other than the positive loop on 2, therefore $\mathscr{G}(f)(0)$ has no cycle passing through 1. Since $f(0) = x^1 = e_1$, by Lemma 5.2, this implies that $\mathscr{G}(f)(x^0)$ has no negative cycle. Now, for any $i \in \{1,\ldots,n-1\}$,

$$\mathscr{G}(f)(x^i) = \sigma(\mathscr{G}(f)(x^{i-1})),$$

where the cyclic permutation $\sigma = (1,2,\ldots,n)$ acts on graphs by permuting vertices. Besides, $\mathscr{G}(f)(y^i) = \mathscr{G}(f)(x^i)$ for any $i \in \{0,\ldots,n-1\}$. We may therefore conclude that for any $x \in C$, $\mathscr{G}(f)(x)$ has no negative cycle. □

6.2. *Antipodal attractive cycles and and-or-nets*

Despite these constraints, we have been able to prove the existence of a local negative cycle under the strong hypothesis of an antipodal attractive cycle, and for a special class of Boolean networks, and-or-nets, introduced in Richard and Ruet (2013).

Definition (and-or-net). A map $\varphi : \mathbb{B}^n \to \mathbb{B}$ is called an *and-map* when it is a product of literals, i.e. there exist disjoint sets P and $N \subseteq \{1,\ldots,n\}$ such that

$$\varphi(x) = \prod_{i \in P} x_i \prod_{i \in N} (x_i + 1),$$

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

with the convention that the empty product is 1. Recall that a map $\varphi : \mathbb{B}^n \to \mathbb{B}$ is said to be a clause when it is a disjunction of literals, i.e. there exist disjoint sets P and $N \subseteq \{1,\dots,n\}$ such that

$$\varphi(x) = \bigvee_{i\in P} x_i \vee \bigvee_{i\in N} (x_i + 1),$$

where $\vee$ denotes supremum and the empty supremum is 0. In both cases, vertices in P (resp. in N) are called the *positive (resp. negative) inputs* of φ. A map $f : \mathbb{B}^n \to \mathbb{B}^n$ is then called an *and-or-net* when for each $i \in \{1,\dots,n\}$, f_i is either an and-map or a clause.

Definition (delocalizing triple). Given an and-or-net f, let V_1, V_2 be the partition of $\{1,\dots,n\}$ such that $i \in V_1$ if and only if f_i is an and-map. Let C be a cycle of $\mathscr{G}(f)$, and $i,j,k \in \{1,\dots,n\}$. Then (i,j_1,j_2) is said to be a *delocalizing triple* of C when j,k are distinct vertices of C and $(i,s_1,j_1),(i,s_2,j_2)$ are two edges of $\mathscr{G}(f)$ that are not in C and such that

$$s_1 \neq s_2 \text{ if } j_1, j_2 \in V_1 \text{ or } j_1, j_2 \in V_2,$$
$$s_1 = s_2 \text{ in all other cases.}$$

A delocalizing triple (i,j_1,j_2) of C is said to be *internal* when i is a vertex of C, *external* otherwise.

The following property, proved in Richard and Ruet (2013), shows that, for and-or-nets, the absence of delocalizing triples for a given cycle is equivalent to being local.

Proposition 6.1. Let $f : \mathbb{B}^n \to \mathbb{B}^n$ be an and-or-net. Given a cycle C of $\mathscr{G}(f)$, C has no delocalizing triple in $\mathscr{G}(f)$ if and only if it is local.

We may now prove that, for and-or-nets, an antipodal attractive cycle implies the existence of a local negative cycle.

Theorem 6.2. Let $f : \mathbb{B}^n \to \mathbb{B}^n$ be an and-or-net. If $\Gamma(f)$ has an antipodal attractive cycle, then $\mathscr{G}(f)$ has a local negative cycle.

Proof. Assume $\Gamma(f)$ has an antipodal attractive cycle

$$\theta = (x^0 \to x^1 \to \cdots \to x^{p-1} \to y^0 \to y^1 \to \cdots \to y^{p-1} \to x^0).$$

We first prove that $\mathscr{G}(f)$ has a negative cycle. To this end, observe that for any $i \in \{0,\dots,p-1\}$, $d(x^i, f(x^i)) = 1$, hence $f(x^i) = x^i + e_{\varphi(i)}$ for some map φ from $\{0,\dots,p-1\}$ to $\{1,\dots,n\}$. Similarly, $f(y^i) = y^i + e_{\varphi(i)}$ because, by definition of an antipodal attractive cycle, y^j is the first return of x^j for all j. Therefore, $\mathscr{G}(f)(x^i)$ and $\mathscr{G}(f)(y^i)$ both have an edge from $\varphi(i)$ to $\varphi(i+1)$, where indices are modulo p, and

$$C = (\varphi(0) \to \varphi(1) \to \cdots \to \varphi(p-1) \to \varphi(0))$$

is an elementary cycle of $\mathscr{G}(f)$. Since $x^0_{\varphi(0)} \neq y^0_{\varphi(0)}$ and

$$f_{\varphi(0)}(x^0) + x^0_{\varphi(0)} = f_{\varphi(0)}(y^0) + y^0_{\varphi(0)} \neq 0,$$

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

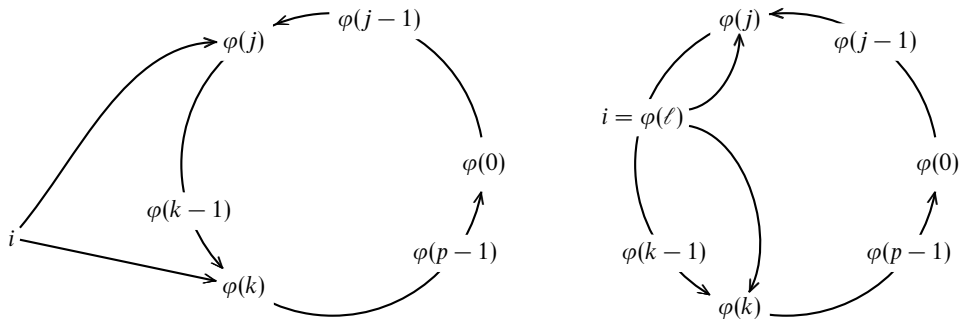


Fig. 2. Proof of Theorem 6.2: the negative elementary cycle C and its assumed (external or internal) delocalizing triple $(i, \varphi(j), \varphi(k))$.

either $x^0_{\varphi(0)} < x^1_{\varphi(0)}$ and $y^0_{\varphi(0)} > y^1_{\varphi(0)}$, or $x^0_{\varphi(0)} > x^1_{\varphi(0)}$ and $y^0_{\varphi(0)} < y^1_{\varphi(0)}$. In either case, the number of direction changes (an increase followed by a decrease, or *vice versa*) between x^0 and y^1 in θ is odd. Consequently, C is a negative elementary cycle of $\mathscr{G}(f)$.

Let us now prove that C is local. According to Proposition 6.1, assume for a contradiction that C has a delocalizing triple $(i, \varphi(j), \varphi(k))$, with $i \in \{1, \ldots, n\}$ and $j, k \in \{0, \ldots, p-1\}$. By symmetry of the definition of a delocalizing triple, we may assume without loss of generality that $j < k$. See Figure 2.

As $\varphi(k)$, which is, by definition of an attractive cycle, the unique degree of freedom of x^k, is not a degree of freedom of x^{k-1},

$$\varphi(k-1) \to \varphi(k)$$

is an edge of $\mathscr{G}(f)(x^k)$, and as θ is antipodal, it is an edge of $\mathscr{G}(f)(y^k)$ as well. For the same reason,

$$\varphi(j-1) \to \varphi(j)$$

is an edge of $\mathscr{G}(f)(x^j)$ and $\mathscr{G}(f)(y^j)$. Now, by definition of a delocalizing triple, one of the two edges

$$\varphi(j-1) \to \varphi(j) \text{ and } \varphi(k-1) \to \varphi(k)$$

of C is not an edge of $\mathscr{G}(f)(x)$ for any $x \in \mathbb{B}^n$ such that $x_i = 0$, and the other edge is not an edge of $\mathscr{G}(f)(x)$ for any $x \in \mathbb{B}^n$ such that $x_i = 1$. In particular, if $\varphi(j-1) \to \varphi(j)$ is an edge of $\mathscr{G}(f)(x)$ and $\varphi(k-1) \to \varphi(k)$ is an edge of $\mathscr{G}(f)(y)$, then $x_i \neq y_i$.

This implies that $(x^j)_i \neq (x^k)_i$. As a consequence, $(i, \varphi(j), \varphi(k))$ is an internal delocalizing triple: $i = \varphi(\ell)$ for some $\ell \in \{0, \ldots, p-1\}$, and moreover, ℓ is either j itself or on the open trajectory from j to k in C: $\ell \in \{j\} \cup C(j,k)$. But then $\ell \notin \{k\} \cup C(k,j)$, hence $(x^k)_i = (y^j)_i$, and we have a contradiction with the fact that $\varphi(j-1) \to \varphi(j)$ is an edge of $\mathscr{G}(f)(y^j)$. □

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

The hypothesis that θ is antipodal cannot be simply avoided in the above proof: it is the reason for the symmetric roles played by the trajectories from j to k and from k to j in C.

The above proof is also obviously very specific to and-or-nets and does not generalize to arbitrary Boolean networks. However, arbitrary Boolean networks can be encoded into and-or-nets (with more vertices), by expressing the underlying Boolean maps f_i in conjunctive normal forms for instance. It is therefore possible that a weak notion of delocalizing triple enables to extend Theorem 6.2 to more general Boolean networks.

Acknowledgments

The author wishes to thank the anonymous reviewer for numerous remarks, as well as Claudine Chaouiya, Elisabeth Remy and El Houssine Snoussi for their invitation to present this work at the meeting on 'Logical formalism, gains and challenges for the modelling of regulatory networks' held in Rabat (Marocco) in April 2011.

Appendix A. Invertibility and Jabobian Matrix

The Jacobian conjecture asserts that if a polynomial complex map $f : \mathbb{C}^n \to \mathbb{C}^n$ has all its Jacobian matrices invertible, then f is bijective. See Bass *et al.* (1982). This appendix shows that, for Boolean maps $f : \mathbb{B}^n \to \mathbb{B}^n$, there is no obvious relationship between the invertibility of the Jacobian matrices $\mathscr{J}(f)(x)$ and the bijectivity of f, an observation which is used in Section 6.1. In particular, the analogue of the Jacobian conjecture for Boolean maps does not hold.

This is to be contrasted with the theorem of Shih and Dong (2005), which can be viewed as a Boolean version of the fixed point conjecture of Cima *et al.* (1999) for maps $\mathbb{C}^n \to \mathbb{C}^n$ (or $\mathbb{R}^n \to \mathbb{R}^n$), a conjecture equivalent to the Jacobian conjecture, as it is proved in Cima *et al.* (1999).

Theorem A.1. Let $f : \mathbb{B}^n \to \mathbb{B}^n$.

i. The fact that f is bijective does not imply that for each $x \in \mathbb{B}^n$, $\mathscr{J}(f)(x)$ is invertible.
ii. The fact that f is hereditarily bijective does not imply that for each $x \in \mathbb{B}^n$, $\mathscr{J}(f)(x)$ is invertible.

Proof. The first claim is a consequence of the second one. To prove the second claim, observe that the asynchronous dynamics $\Gamma(f)$ of the map $f : \mathbb{B}^3 \to \mathbb{B}^3$ defined by

$$f_1(x) = x_1 + (x_2 + 1)x_3$$
$$f_2(x) = x_2 + (x_3 + 1)x_1$$
$$f_3(x) = x_3 + (x_1 + 1)x_2,$$

consists in two fixed points $(0,0,0)$ and $(1,1,1)$ and three attractive cycles of length 2. This shows that the map f is a bijection whose orbits are either fixed points or pairs $\{x, x + e_i\}$ of points which are 1-distant from each other. Since this property is stable

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

under projection, f is also hereditarily bijective. However,

$$\mathscr{J}(f)(x) = \begin{pmatrix} 1 & x_3 & x_2+1 \\ x_3+1 & 1 & x_1 \\ x_2 & x_1+1 & 1 \end{pmatrix},$$

hence $\mathscr{J}(f)(0)$, a matrix whose sum of three columns equals 0, is not invertible. □

Theorem A.2. Let $f : \mathbb{B}^n \to \mathbb{B}^n$.

i. The fact that for each $x \in \mathbb{B}^n$, $\mathscr{J}(f)(x)$ is invertible does not imply that $f : \mathbb{B}^n \to \mathbb{B}^n$ is bijective.
ii. The fact that for each $x \in \mathbb{B}^n$, $\mathscr{I} + \mathscr{J}(f)(x)$ is nilpotent does not imply that $f : \mathbb{B}^n \to \mathbb{B}^n$ is bijective.

Proof. The first claim is a consequence of the second one. To prove the second claim, let $f : \mathbb{B}^3 \to \mathbb{B}^3$ be defined by $f_i(x) = x_i + x_1x_2 + x_2x_3 + x_3x_1$ for $i = 1, 2, 3$: then f is not bijective because $f(0,0,0) = f(1,1,1) = (0,0,0)$, but

$$\mathscr{I} + \mathscr{J}(f)(x) = \begin{pmatrix} x_2+x_3 & x_3+x_1 & x_1+x_2 \\ x_2+x_3 & x_3+x_1 & x_1+x_2 \\ x_2+x_3 & x_3+x_1 & x_1+x_2 \end{pmatrix}$$

is nilpotent of order 2. □

References

Bass, H., Connell, E. H. and Wright, D. (1982) The Jacobian conjecture: Reduction of degree and formal expansion of the inverse. *Bulletin of the American Mathematical Society* **7** (2) 287–330.

Bazsó F. (2000) Derivations of vector-valued Boolean functions. *Acta Mathematica Hungarica* **87** (3) 197–203.

Cima, A., Gasull, A. and Mañosas, F. (1999) The discrete Markus–Yamabe problem. *Nonlinear Analysis* **35** 343–354.

Kauffman, S. A. (1969) Metabolic stability and epigenesis in randomly connected nets. *Journal of Theoretical Biology* **22** 437–467.

Kauffman, S. A. (1993) *The Origins of Order: Self-Organization and Selection in Evolution*, Oxford University Press.

Kim, K. H. (1982) *Boolean Matrix Theory and Applications*, Marcel Dekker.

Remy, E. and Ruet, P. (2007) On differentiation and homeostatic behaviours of Boolean dynamical systems. In: Transactions on Computational Systems Biology. *Springer Lecture Notes in Computer Science* **4780** 92–101.

Remy, E., Ruet, P. and Thieffry, D. (2008) Graphic requirements for multistability and attractive cycles in a Boolean dynamical framework. *Advances in Applied Mathematics* **41** (3) 335–350.

Richard, A. (2010) Negative circuits and sustained oscillations in asynchronous automata networks. *Advances in Applied Mathematics* **44** (4) 378–392.

Richard, A. and Ruet, P. (2013) From kernels in directed graphs to negative cycles in Boolean networks. *Discrete Applied Mathematics* **161** 1106–1117.

Robert, F. (1995) *Les Systèmes Dynamiques Discrets*, Mathématiques et Applications, volume 19, Springer.

Rudeanu, S. (1974) *Boolean Functions and Equations*, North-Holland.

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press

Shih, M.-H. and Dong, J.-L. (2005) A combinatorial analogue of the Jacobian problem in automata networks. *Advances in Applied Mathematics* **34** (1) 30–46.

Thomas, R. (1973) Boolean formalization of genetic control circuits. *Journal of Theoretical Biology* **42** 563–585.

Thomas, R. (1981) On the relation between the logical structure of systems and their ability to generate multiple steady states and sustained oscillations. In: *Series in Synergetics*, volume 9, Springer 180–193.

Thomas, R. and Kaufman, M. (2001) Multistationarity, the basis of cell differentiation and memory. i. Structural conditions of multistationarity and other non-trivial behaviour. *Chaos* **11** 170–179.

von Neumann, J. (1966) *Theory of Self-Reproducing Automata*, University of Illinois Press.

https://doi.org/10.1017/S096012951400036X Published online by Cambridge University Press