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Abstract

Given a digraph G , a lot of attention has been deserved on the maximum number $\phi(G)$ of fixed points in a Boolean network $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ with G as interaction graph. In particular, a central problem in network coding consists in studying the optimality of the classical upper bound $\phi(G) \leq 2^\tau$, where τ is the minimum size of a feedback vertex set of G . In this paper, we study the maximum number $\phi_m(G)$ of fixed points in a *monotone* Boolean network with interaction graph G . We establish new upper and lower bounds on $\phi_m(G)$ that depends on the cycle structure of G . In addition to τ , the involved parameters are the maximum number ν of vertex-disjoint cycles, and the maximum number ν^* of vertex-disjoint cycles verifying some additional technical conditions. We improve the classical upper bound 2^τ by proving that $\phi_m(G)$ is at most the largest sub-lattice of $\{0, 1\}^\tau$ without chain of size $\nu + 1$, and without another forbidden-pattern of size $2\nu^*$. Then, we prove two optimal lower bounds: $\phi_m(G) \geq \nu + 1$ and $\phi_m(G) \geq 2^{\nu^*}$. As a consequence, we get the following characterization: $\phi_m(G) = 2^\tau$ if and only if $\nu^* = \tau$. As another consequence, we get that if c is the maximum length of a chordless cycle of G then $2^{\nu/3^c} \leq \phi_m(G) \leq 2^{c\nu}$. Finally, with the technics introduced, we establish an upper bound on the number of fixed points of any Boolean network according to its signed interaction graph.

1 Introduction

A *Boolean network* with n components is a discrete dynamical system usually defined by a global transition function

$$f : \{0, 1\}^n \rightarrow \{0, 1\}^n, \quad x = (x_1, \dots, x_n) \mapsto f(x) = (f_1(x), \dots, f_n(x)).$$

Boolean networks have many applications. In particular, since the seminal papers of McCulloch and Pitts [19], Hopfield [14], Kauffman [15, 16] and Thomas [26, 27], they are omnipresent in the modeling of neural and gene networks (see [5, 17] for reviews). They are also essential tools in information theory, for the network coding problem [1, 8].

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The structure of a Boolean network f is usually represented via its *interaction graph*, which is the digraph G with vertex set $\{1, \dots, n\}$ that contains an arc uv if f_v depends on x_u (G may have *loops*, that is, arcs from a vertex to itself).

In many contexts, as in molecular biology, the first reliable informations are represented under the form of an interaction graph, while the actual dynamics are very difficult to observe [28, 17]. A natural question is then the following: *What can be said about f according to G only?* Among the many dynamical properties that can be studied, fixed points are of special interest, since they correspond to stable states and often have a strong meaning. For instance, in the context of gene networks, they correspond to stable patterns of gene expression at the basis of particular biological processes [27, 2]. As such, they are arguably the property which has been the most thoroughly studied. The study of the number of fixed points and its maximization in particular is the subject of a stream of work, e.g. in [24, 22, 3, 10, 4, 9].

Given a digraph G , let $\phi(G)$ be the maximum number of fixed points in a Boolean network whose interaction graph is (isomorphic to) G , and let $\phi'(G)$ be the maximum number of fixed points in a Boolean network whose interaction graph is (isomorphic to) a subgraph of G . A fundamental result is the following “classical” upper bound, proved independently in different contexts in [23, 3]:

$$\phi(G) \leq \phi'(G) \leq 2^\tau$$

where $\tau = \tau(G)$ is the *transversal number* of G , that is, the minimum size of a set of vertices intersecting every cycle of G (cycles are always directed and without “repeated vertices”). The optimality of this bound is a central problem in network coding: the so called *binary network coding problem* consists in deciding if $\phi'(G) = 2^\tau$ [23, 10]. Concerning lower bounds, let us mention the following “folklore” lower bound

$$2^\nu \leq \phi'(G)$$

where $\nu = \nu(G)$ is the *packing number* of G , that is, the maximum number of vertex-disjoint cycles in G (we have, obviously, $\nu \leq \tau$). Curiously, there are, up to our knowledge, no lower bounds on $\phi(G)$. See [10] for other upper and lower bounds on $\phi'(G)$ based on other graph parameters.

In this paper we study fixed points in *monotone* Boolean networks, that is, functions $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ such that

$$\forall x, y \in \{0, 1\}^n, \quad x \leq y \Rightarrow f(x) \leq f(y).$$

Given a digraph G , we denote by $\phi_m(G)$ the maximum number of fixed points in a monotone Boolean network whose interaction graph is (isomorphic to) G , and we denote by $\phi'_m(G)$ the maximum number of fixed points in a monotone Boolean network whose interaction graph is (isomorphic to) a subgraph of G . Our main results, summarized below, are upper and lower bounds $\phi_m(G)$ and applications of the technics introduced for these bounds to the more general context of signed digraphs.

We cannot speak about fixed points in monotone Boolean networks without first mention the well-known Knaster-Tarski theorem, the following: *The set of fixed points of a monotone Boolean network f is a non-empty lattice.* This statement does not involved the interaction graph of f , and we will show how to use this graph in order to obtain additional information on the structure of the lattice of fixed points (and in particular on the maximal chains it contains). This is essentially from this additional information that our upper-bounds on $\phi_m(G)$ are derived.

1.1 Results

1.1.1 Upper bounds

Our first result is that, given a monotone Boolean network f with interaction graph G , the set of fixed points of f is isomorphic to a lattice $L \subseteq \{0, 1\}^\tau$ without chain of size $\nu + 1$. By a well known theorem of Erdős [6], the maximal size of such a lattice is exactly two plus the sum of the $\nu - 1$ largest binomial coefficients $\binom{\tau}{k}$. We thus obtain the following bound, which improve the classical one when the gap between ν and τ is large:

$$\phi_m(G) \leq 2 + \sum_{k=\lfloor \frac{\tau-\nu+2}{2} \rfloor}^{\lfloor \frac{\tau+\nu-2}{2} \rfloor} \binom{\tau}{k}.$$

From this bound we recover the implication $\phi_m(G) = 2^\tau \Rightarrow \nu = \tau$ already established in [8] with a dedicated proof. Since $2^\nu \leq \phi'_m(G)$ (this is an easy exercise), we deduce that

$$\phi'_m(G) = 2^\tau \iff \nu = \tau$$

and this solves the binary network coding problem in the monotone case.

Then, we refine the upper bound by introducing another graph parameters, ν^* , defined as follows. Let C_1, \dots, C_k be a *packing* of size k , that is, is a collection of k vertex-disjoint cycles. A path P is said *principal* if no arcs and no internal vertices of P belong to the packing. We say that the packing is *special* if the following holds: for every cycle C_i and every vertex v in C_i , if there exists a principal path from a cycle $C_j \neq C_i$ to v , then there exists a principal path from C_i or a source to v (a *source* is a vertex of in-degree zero). We then define $\nu^* = \nu^*(G)$ as the maximum size of a special packing of G (we have, obviously, $\nu^* \leq \nu$). Also, we say that a subset $X \subseteq \{0, 1\}^n$ has a *special k -pattern* if there exists a subset $S \subseteq X$ of size k such that $1 - x \in S$ for all $x \in S$, and $x \leq 1 - y$ for all distinct $x, y \in S$. Our refinement is based on the following fact: the set of fixed points of f is isomorphic to a lattice $L \subseteq \{0, 1\}^\tau$ without special $(\nu^* + 1)$ -pattern. This has several consequences that we will discuss. In particular, since $\{0, 1\}^\tau$ has a τ -pattern, we deduce that $\phi_m(G) = 2^\tau \Rightarrow \nu^* = \tau$. Since $\nu^* \leq \nu \leq \tau$, this improves the implication $\phi_m(G) = 2^\tau \Rightarrow \nu = \tau$ mentioned above.

1.1.2 Lower bounds

Next, we prove several lower bounds by construction. The first is

$$\nu + 1 \leq \phi_m(G)$$

and is optimal for every possible value of ν . Since $2^\nu \leq \phi'_m(G)$, this optimality is not obvious a priori. Actually, we will prove that $\phi_m(G) = \nu + 1$ if G is of maximal in-degree at most two and if G has an arc between any two vertex-disjoint cycles.

The second lower bound is

$$2^{\nu^*} \leq \phi_m(G)$$

and is also optimal for every possible value of ν^* (consider for instance digraphs that consist in disjoint cycles). As a consequence, if $\nu^* = \tau$ then $\phi_m(G) = 2^\tau$ and since, as seen above, the converse is true we have the following characterization, showing that the introduction of ν^* really makes sense:

$$\phi_m(G) = 2^\tau \iff \nu^* = \tau.$$

Finally we will prove, using both the lower bound 2^{ν^*} and a result on dominating sets in digraphs, that if G has k vertex-disjoint cycles of length at most ℓ then $2^{k/3^\ell} \leq \phi_m(G)$. Hence,

if $c = c(G)$ denotes the *circumference* of G , that is the maximum length of a chordless cycle of G , then $2^{\nu/3^c} \leq \phi_m(G)$, and since $\tau \leq c\nu$ this gives

$$2^{\nu/3^c} \leq \phi_m(G) \leq 2^{c\nu}.$$

Hence, if G is symmetrical and loop-less, and thus identifiable with an undirected simple graph, then $2^{\nu/9} \leq \phi_m(G)$, and we will prove that the 9 can be replaced by a 6. More precisely, we will prove that $\nu/6 \leq \nu^*$ from which we immediately get $2^{\nu/6} \leq \phi_m(G)$.

1.1.3 Upper bound for signed digraphs

Our motivation for studying fixed points in monotone Boolean networks comes from the studies of the relationships between the fixed points of Boolean network $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ and its *signed* interaction graph, which play a predominant role in biological and sociological applications [27, 28, 12].

Formally, the *signed interaction graph* of f is obtained by associating to its interaction graph G the arc-labeling function σ defined for all arc uv as follows:

$$\sigma(uv) = \begin{cases} 1 & \text{if } f_v(x) \leq f_v(x + e_u) \text{ for all } x \in \{0, 1\}^n \text{ with } x_u = 0, \\ -1 & \text{if } f_v(x) \geq f_v(x + e_u) \text{ for all } x \in \{0, 1\}^n \text{ with } x_u = 0, \\ 0 & \text{otherwise.} \end{cases}$$

(where e_u denotes the point of $\{0, 1\}^n$ where all the components are zeroes, excepted the one indexed by u). The *sign of a cycle* is the product of the sign of its arcs. Note that f is monotone if and only if all the arcs are labeled positive. If (G, σ) is a signed digraph then $\phi(G, \sigma)$ denotes the maximum number of fixed points in a Boolean network with a signed interaction graph isomorphic to (G, σ) . Let $\tau^+ = \tau^+(G, \sigma)$ be the minimum size of a set of vertices intersecting every non-negative cycle of (G, σ) .

The biologist Thomas put the emphasis on the dual role of positive and negative cycles, roughly: positive cycles are the key ingredients for fixed points multiplicity, and negative cycles for some kind of sustained oscillations [27, 28]. One of the authors of this paper proved the following upper bound, that generalizes the classic one, and that gives a strong support of the idea of Thomas concerning positive cycles [3]:

$$\phi(G, \sigma) \leq 2^{\tau^+}.$$

The optimality of this bound is a difficult problem, and we think that it could be improved by taking, in some way, information on negative cycles. This was our initial motivation. For that problem, it is natural to study the extreme case where all cycles are positive, and this essentially corresponds to the monotone case. Indeed, as explained latter, if (G, σ) is a strongly connected signed digraph with only positive cycles then $\phi(G, \sigma) = \phi_m(G)$ and all the previous results apply¹.

Actually, using tools introduced to bound $\phi_m(G)$ we will establish an upper bound that works for every signed digraph and which is competitive with 2^{τ^+} . Let us say that (G, σ) and (G, σ') are *equivalent* if there exists a set of vertices I such that, for every arc uv : $\sigma'(uv) = \sigma(uv)$ if $u, v \in I$ or $u, v \notin I$; and $\sigma'(uv) = -\sigma(uv)$ otherwise. Let us say that a *monotone feedback vertex set* of (G, σ) is a feedback vertex set I of G such that every non-positive arc of (G, σ) has its final vertex in I . Let $\tilde{\tau}_m = \tilde{\tau}_m(G, \sigma)$ the minimum size of a monotone feedback vertex set

¹If (G, σ) has only positive cycles and G is not strongly connected, then we may have $\phi(G, \sigma) > \phi_m(G)$. Thus the strong connectivity is necessary to ensure the equality.

in a signed digraph equivalent to (G, σ) . We will prove that $\phi(G, \sigma)$ is at most the sum of the $\nu^+ + 1$ largest binomial coefficient $\binom{\tilde{\tau}_m}{k}$, where ν^+ is the maximum number of vertex-disjoint non-negative cycles in (G, σ) . In other words, for every signed digraph (G, σ) ,

$$\phi(G, \sigma) \leq \sum_{k=\lfloor \frac{\tilde{\tau}_m - \nu^+}{2} \rfloor}^{\lfloor \frac{\tilde{\tau}_m + \nu^+}{2} \rfloor} \binom{\tilde{\tau}_m}{k}.$$

This improves the bound 2^{τ^+} when $\tilde{\tau}_m = \tau^+$ and when the gap between ν^+ and $\tilde{\tau}_m$ is large. This holds, for instance, if G is obtained from the complete graph by replacing each edge by a directed cycle of length two and if $\sigma = \text{cst} = -1$. In that case $\tilde{\tau}_m = \tau = \tau^+$ and $\nu^+ = \lfloor \frac{\tau+1}{2} \rfloor$.

1.2 Notations and basic definitions

Unless otherwise specified, all the cycles and paths we consider are always directed and without repeated vertices, excepted that in a path $P = v_0 v_1 \dots v_\ell$ we may have $v_0 = v_\ell$ (and, in that case, the path is actually a cycle). The vertices $v_1, \dots, v_{\ell-1}$, if they exist, are the *internal vertices* of P . A *chord* in a cycle C is an arc uv such that u and v are in C but not uv . A *loop* is an arc from a vertex to itself (a cycle of length one). Given a digraph $G = (V, A)$, the subgraph of G induced by a set $I \subseteq V$ is denoted $G[I]$ and $G \setminus I = G[V \setminus I]$. A *feedback vertex set* is a set of vertices I such that $G \setminus I$ is acyclic. Thus $\tau = \tau(G)$ is the minimum size of a feedback vertex set of G . A *strongly connected component* is a set of vertices $S \subseteq V$ such that $G[S]$ is strongly connected and such that S is maximal for this property (with respect to the inclusion). The set of in-neighbors of a vertex v is denoted $N_G^-(v)$ (and $v \in N_G^-(v)$ if there is a loop on v). The in-degree of v is $|N_G^-(v)|$. A *source* is a vertex of in-degree zero.

For every positive integer n we set $[n] = \{1, \dots, n\}$. We see $\{0, 1\}^n$ has the n -dimensional Boolean lattice, and every subset $X \subseteq \{0, 1\}^n$ is seen as a poset with the usual partial order \leq (i.e. $x \leq y$ if and only if $x_i \leq y_i$ for all $i \in [n]$). Hence, two subsets $X, Y \subseteq \{0, 1\}^n$ are *isomorphic* if there exists a bijection from X to Y preserving the order. If $x \in \{0, 1\}^n$ then $\bar{x} = 1 - x$ is the negation of x (i.e. $\bar{x}_i = 1 - x_i$ for all $i \in [n]$). If $I \subseteq [n]$ then x_I is the restriction of x to the components in I , so that $x_I \in \{0, 1\}^I$. For every $I \subseteq [n]$ we denote by e_I the point of $\{0, 1\}^n$ such that $(e_I)_v = 1$ if and only if $v \in I$. We use e_v as an abbreviation of $e_{\{v\}}$. For all $0 \leq k \leq n$ we set denote by $\binom{[n]}{k}$ the set of $x \in \{0, 1\}^n$ containing exactly k ones.

Let $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$. For all $v \in [n]$, we say that the component $f_v : \{0, 1\}^n \rightarrow \{0, 1\}$ of f is monotone if, for all $x, y \in \{0, 1\}^n$, $x \leq y$ implies $f_v(x) \leq f_v(y)$. Thus f is monotone if and only if all its components are. The main tool to study f is its interaction graph G , whose definition is detailed here: the vertex set of G is $[n]$, and for all $u, v \in [n]$, there is an arc uv if f_v depends on x_u , that is, if there exists $x, y \in \{0, 1\}^n$ that only differ in $x_u \neq y_u$ such that $f_v(x) \neq f_v(y)$. We denote by $\text{FIX}(f)$ the set of fixed points of f .

1.3 Organization

Upper and lower bounds on $\phi_m(G)$ are presented in Section 2 and 3 respectively. Results on signed digraphs are presented Section 4. Concluding remarks are given in Section 5.

2 Upper bound for monotone networks

2.1 Classical upper bound and isomorphism

The following lemma is a classical result proved in [3] from which we immediately deduce the classical upper bound $\phi(G) \leq 2^\tau$ (it is sufficient to take I such that $|I| = \tau$). Below, we will

refine this lemma under some additional conditions about the monotony of the components of f . Both proofs are almost identical, and to show that explicitly both proofs are presented.

Lemma 1. *Let f be a Boolean network and let I be a feedback vertex set of its interaction graph. Then*

$$\forall x, y \in \text{FIX}(f), \quad x = y \iff x_I = y_I.$$

Proof. The direction \Rightarrow is obvious. To prove the converse, suppose that $x_I = y_I$ and let us prove that $x = y$. Let G be the interaction graph of f and let v_1, \dots, v_m be an enumeration of the vertices of $G \setminus I$ in the topological order (in such a way that there is no arc from v_j to v_i if $i < j$). We prove, by induction on i , that $x_{v_i} = y_{v_i}$. Since f_{v_1} only depends on variables with indices in I we can write $x_{v_1} = f_{v_1}(x) = f_{v_1}(x_I)$ and $y_{v_1} = f_{v_1}(y) = f_{v_1}(y_I)$. Since $x_I = y_I$ we deduce that $x_{v_1} = y_{v_1}$. Now, let $1 < i \leq m$. Then, similarly, f_{v_i} only depends on variables with indices in $J = I \cup \{v_1, \dots, v_{i-1}\}$ and thus we can write $x_{v_i} = f_{v_i}(x) = f_{v_i}(x_J)$ and $y_{v_i} = f_{v_i}(y) = f_{v_i}(y_J)$. By induction hypothesis $x_J = y_J$, thus $x_{v_i} = y_{v_i}$. This proves that $x = y$. \square

Lemma 2. *Let f be a Boolean network and let I be a feedback vertex set of its interaction graph. If f_v is monotone for all $v \notin I$ then*

$$\forall x, y \in \text{FIX}(f), \quad x \leq y \iff x_I \leq y_I.$$

As a consequence, $\text{FIX}(f)$ is isomorphic to $\{x_I : x \in \text{FIX}(f)\}$

Proof. The direction \Rightarrow is obvious. To prove the converse, suppose that $x_I \leq y_I$ and let us prove that $x \leq y$. Let G be the interaction graph of f and let v_1, \dots, v_m be an enumeration of the vertices of $G \setminus I$ in the topological order (in such a way that there is no arc from v_j to v_i if $i < j$). We prove, by induction on i , that $x_{v_i} \leq y_{v_i}$. Since f_{v_1} only depends on variables with an index in I we can write $x_{v_1} = f_{v_1}(x) = f_{v_1}(x_I)$ and $y_{v_1} = f_{v_1}(y) = f_{v_1}(y_I)$. Since f_{v_1} is monotone and $x_I \leq y_I$ we deduce that $x_{v_1} \leq y_{v_1}$. Now, let $1 < i \leq m$. Then, similarly, f_{v_i} only depends on variables with an index in $J = I \cup \{v_1, \dots, v_{i-1}\}$ and we can write $x_{v_i} = f_{v_i}(x) = f_{v_i}(x_J)$ and $y_{v_i} = f_{v_i}(y) = f_{v_i}(y_J)$. Since f_{v_i} is monotone and since, by induction hypothesis, $x_J \leq y_J$, we deduce that $x_{v_i} \leq y_{v_i}$. This proves that $x \leq y$. \square

2.2 Introduction of ν in the upper bound

The next lemma is a simple but very useful (and apparently new) application of a well known theorem, due to one of the authors [3, Theorem 3] (see also Remy-Ruet-Thieffry [22]): *If a Boolean network f has two distinct fixed points x and y , then its signed interaction graph has a non-negative cycle C such that $x_v \neq y_v$ for every vertex v of C .*

Lemma 3. *If the set of fixed points of a Boolean network f contains a chain of size $\ell + 1$, then the signed interaction graph of f has ℓ vertex-disjoint non-negative cycles.*

Proof. Suppose indeed that $x^0 < x^1 < \dots < x^\ell$ is a chain of fixed points of size $\ell + 1$. For all $k \in [\ell]$, let I_k be the set of components that differs between x^{k-1} and x^k . Then, by the theorem mentioned above, for all $k \in [\ell]$, the signed interaction graph of f has a non-negative cycle with only vertices in I_k . Since the set I_1, \dots, I_ℓ are mutually disjoint, this proves the lemma. \square

The following theorem is a straightforward application of the previous lemmas and two well known theorems in combinatorics. The first is the Knaster-Tarski theorem stated in the introduction. The second is a theorem of Erdős [6]: *For every $1 \leq \ell \leq n$, the maximal size of a subset of $\{0, 1\}^n$ without chain of size $\ell + 1$ is the sum of the ℓ largest binomial coefficients $\binom{n}{k}$.*

Theorem 1. *Let f be a monotone Boolean network with interaction graph G . The number of fixed points in f is at most 2 plus the sum of the $\nu - 1$ largest binomial coefficients $\binom{I}{k}$.*

Proof. By the Knaster-Tarski theorem, $\text{FIX}(f)$ is a lattice. By Lemma 2, this lattice is isomorphic to a lattice $L \subseteq \{0, 1\}^\tau$, and by Lemma 3, L has no chain of size $\nu + 2$. Let L' be obtained from L by removing its maximal and minimal element. Since every maximal chain in L contains these two extremal elements, L' has no chain of size ν . It is then sufficient to apply the Erdős' theorem mentioned above. \square

An equivalent statement is the one given in the introduction:

$$\phi_m(G) \leq 2 + \sum_{k=\lfloor \frac{\tau-\nu+2}{2} \rfloor}^{\lfloor \frac{\tau+\nu-2}{2} \rfloor} \binom{\tau}{k}. \quad (1)$$

Hence, if $\phi_m(G) = 2^\tau$ then $\phi_m(G)$ equals 2 plus the sum of the $\tau-1$ largest binomial coefficients of order τ , and thus $\nu-1 \geq \tau-1$. Since $\nu \leq \tau$ this implies $\nu = \tau$. Thus we recover the implication $\phi_m(G) = 2^\tau \Rightarrow \nu = \tau$ established in [8] with a dedicated proof. Another straightforward consequence is:

$$\nu \leq 1 \Rightarrow \phi_m(G) \leq 2. \quad (2)$$

The above upper bound on $\phi_m(G)$ improve the classical upper bound 2^τ when the gap between ν and τ is large. But for a fixed ν , τ cannot be arbitrarily large. This results from the fact that directed cycles have the so called Erdős-Pósa property: as proved by Reed, Roberston, Seymour and Thomas [21], there exists a smallest function $h : \mathbb{N} \rightarrow \mathbb{N}$ such that $\tau \leq h(\nu)$ for every digraph G . The only known exact value of h is $h(1) = 3$ [20], and [21] provides an upper bound on $h(\nu)$ which is of power tower type. It is however difficult to find family of digraphs for which the gap between ν and τ is large. To our knowledge, the best construction is by Seymour [25], who shows that for n sufficiently large there exists a digraph on $2n$ vertices with $\tau \geq \frac{1}{30}\nu \log \nu$. Let us also mention that $\nu = \tau$ for every strongly planar digraph [11]. These subtle relationships between ν and τ make particularly hard the study of the optimality of the upper bound on $\phi_m(G)$.

We will now identify another structure in $\text{FIX}(f)$ that forces the presence of disjoint cycles. We need the following definition.

Definition 1. A k -pattern in a subset $P \subseteq \{0, 1\}^n$ is a couple of two sequences (x^1, \dots, x^k) and (y^1, \dots, y^k) , each containing k distinct elements of P , such that, for all $p, q \in [k]$,

$$x^p \leq y^q \iff p \neq q.$$

For instance, the n base vectors (e_1, \dots, e_n) and their negations $(\bar{e}_1, \dots, \bar{e}_n)$ forms an n -pattern of $\{0, 1\}^n$. Also, if $x \in \{0, 1\}^n$ and $x \neq 0$, then (x, \bar{x}) and (\bar{x}, x) form a 2-pattern of $\{0, 1\}^n$. This shows that the two sequences may have common elements. Additional properties on k -patterns are given below.

Proposition 1. If $X = (x^1, \dots, x^k)$ and $Y = (y^1, \dots, y^k)$ form a k -pattern of $\{0, 1\}^n$, then X and Y are antichains and $k \leq n$.

Proof. There is nothing to prove if $k = 1$ so assume that $k \geq 2$. If $x^p \leq x^q$ for some $p \neq q$ then $x^p \leq x^q \leq y^p$, which is a contradiction. Thus X is an antichain, and we prove similarly that Y is an antichain. Let us prove now that $k \leq n$. For all $p \in [k]$ there exists at least one $v \in [n]$ such that $x_v^p = 1$ since otherwise $x^p \leq y^p$. Furthermore, if $x_v^p = 1$ and $x_v^q = 1$ for some $q \neq p$ then $y_v^p = 1$ since $x^q \leq y^p$. Thus, if for all v such that $x_v^p = 1$ there exists some $q \neq p$ with $x_v^q = 1$ then $x^p \leq y^p$, a contradiction. Thus there exists at least one $v \in [n]$, denote it as v_p , such that $x_{v_p}^p > x_{v_p}^q$ for all $q \neq p$. Thus the v_p are all distinct and we deduce that $k \leq n$. \square

Lemma 4. *Let f be a monotone network with interaction graph G . If the set of fixed points of f has a k -pattern, then G has k vertex-disjoint cycles.*

Proof. Suppose that (x^1, \dots, x^k) and (y^1, \dots, y^k) form a k -pattern in $\text{FIX}(f)$. For every $p \in [k]$ let V_p be the set of vertices v in G such that $x_v^p > y_v^p$. This set V_p is not empty since $x^p \not\leq y^p$. Furthermore, if $v \in V_p$, then $f_v(x^p) = x_v^p > y_v^p = f_v(y^p)$ and since f_v is monotone, we deduce that G has an arc uv with $x_u^p > y_u^p$. Thus $G[V_p]$ has minimal in-degree at least one, and thus $G[V_p]$ has a cycle, say C_p . Let us prove that the k cycles C_1, \dots, C_k selected in this way are vertex-disjoint. Let $p, q \in [k]$ with $p \neq q$. If $v \in V_p$ then $x_v^p > y_v^p$ and since $y^p \geq x^q$ we have $x_v^q = 0$ and thus $v \notin V_q$. Hence $V_p \cap V_q = \emptyset$, thus C_p and C_q are indeed vertex-disjoint. \square

Suppose that f has 2^τ fixed points. Then $\text{FIX}(f)$ is isomorphic to $\{0, 1\}^\tau$, which has a τ -pattern. Thus, according to the previous lemma, we have $\nu = \tau$ and we recover, by another way, the implication $\phi_m(G) = 2^\tau \Rightarrow \nu = \tau$. Furthermore, we deduce from the previous lemma that $\{0, 1\}^\tau$ has no $(\tau + 1)$ -pattern (since otherwise $\nu > \tau$ which is false). This has been proved independently in Proposition 1.

2.3 Introduction of ν^* in the upper bound

We will now identify a slightly different structures that force the presence of disjoint cycles verifying some additional conditions. These structures are the *special k -patterns*, define in a compact way in the introduction. Here is an alternative and more explicit definition, based on k -patterns.

Definition 2. *A k -pattern $(x^1, \dots, x^k), (y^1, \dots, y^k)$ is special if, for all $p \in [k]$,*

$$y^p = \overline{x^p}.$$

For instance, the n base vectors (e_1, \dots, e_n) and their negations $(\overline{e_1}, \dots, \overline{e_n})$ forms a special n -pattern. This example can be generalized as follows. For every $1 \leq \ell \leq \frac{n}{2}$ there always exists a collection I_1, \dots, I_k of $k = \lfloor \frac{n}{\ell} \rfloor$ disjoint subsets of $[n]$ of size ℓ . The sequences $(e_{I_1}, \dots, e_{I_k})$ and $(\overline{e_{I_1}}, \dots, \overline{e_{I_k}})$ then form a special k -pattern. As a consequence, for every $P \subseteq \{0, 1\}^n$,

$$\binom{[n]}{\ell} \subseteq P \text{ and } \binom{[n]}{n-\ell} \subseteq P \Rightarrow P \text{ has a special } \lfloor \frac{n}{\ell} \rfloor\text{-pattern.} \quad (3)$$

Conversely, every special k -pattern can obviously be expressed as $(e_{I_1}, \dots, e_{I_k}), (\overline{e_{I_1}}, \dots, \overline{e_{I_k}})$ for some subsets I_1, \dots, I_k of $[n]$. Then, necessarily, these sets I_p are pairwise disjoint, since for all distinct $p, q \in [k]$, we have $e_{I_p} \leq \overline{e_{I_q}}$ and this is equivalent to $I_p \subseteq [n] \setminus I_q$. Note also that if there exists $x \in P$ such that $\overline{x} \in P$ then P has a special 2-pattern, formed by (x, \overline{x}) and (\overline{x}, x) , and conversely, if P has a special 2-pattern then, by definition, there exists $x \in P$ such that $\overline{x} \in P$. Thus, setting $\overline{P} = \{\overline{x} : x \in P\}$, we have

$$P \text{ has no special 2-patterns} \iff P \cap \overline{P} = \emptyset. \quad (4)$$

We also recall, from the introduction, the definition of a *principal path* and a *special packing*.

Definition 3. *A packing of size k in a digraph G is a collection of k vertex-disjoint cycles of G , say C_1, \dots, C_k . Given such a packing, a path P of G is said principal if it has no arcs and no internal vertices that belong to some cycle of the packing². We say that the packing is special if the following holds: for every cycle C_i and for every vertex v in C_i , if there exists a principal path from a cycle $C_j \neq C_i$ to v , then there exists a principal path from C_i or from a source to v . We denote by $\nu^* = \nu^*(G)$ the maximum size of a special packing in G .*

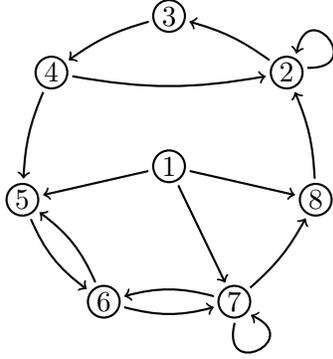
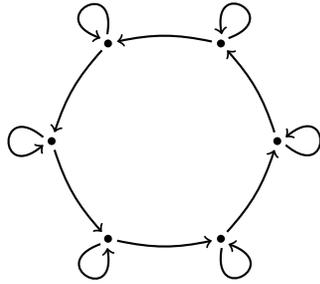
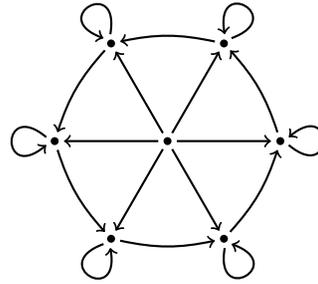


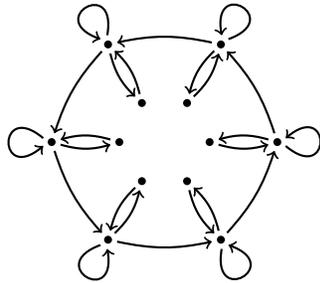
Figure 1: The cycles $C_1 = 2, 3, 4, 2$, $C_2 = 5, 6, 5$ and $C_3 = 7, 7$ form a packing which is not special: $P = 7, 6$ is a principal path from C_3 to 6, but there are no principal paths from C_2 to 6 or from a source to 6. However, the packing formed by C_1 and C_2 is a special packing. Indeed, $P = 6, 7, 8, 2$ is the unique principal path from C_2 to C_1 , and $P' = 2, 2$ is a principal path from C_1 to 2. Furthermore, $P = 5, 4$ is the unique principal path from C_1 to C_2 and there exists a principal path $P' = 1, 5$ from a source to 5.



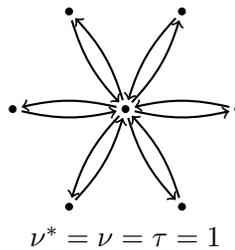
$$\nu^* = \lfloor n/2 \rfloor \quad \nu = \tau = n$$



$$\nu^* = \nu = \tau = n - 1.$$



$$\nu^* = \nu = \tau = n/2$$



$$\nu^* = \nu = \tau = 1$$

Figure 2: Parameters ν^* , ν and τ for some digraphs.

We now connect special patterns with special packings in the following way.

Lemma 5. *Let f be a monotone network with interaction graph G , and let I be a feedback vertex set of G . If $\{x_I : x \in \text{FIX}(f)\}$ has a special k -pattern, then G has a special packing of size k .*

Proof. Let $X = (x^1, \dots, x^k)$ and $Y = (y^1, \dots, y^k)$ be two sequences of k distinct fixed points of f , and suppose that $X_I = (x_I^1, \dots, x_I^k)$ and $Y_I = (y_I^1, \dots, y_I^k)$ form a special k -pattern of $L = \{x_I : x \in \text{FIX}(f)\}$. Since, by Lemma 2, $\text{FIX}(f)$ and L are isomorphic, X and Y form a k -pattern of $\text{FIX}(f)$ (which is, however, not necessarily special).

For every $p \in [k]$ we set

$$V_p = \{v : x_v^p > y_v^p\} \quad \text{and} \quad U_p = \{v : x_v^p \geq y_v^p\}.$$

We first prove that, for all distinct $p, q \in [k]$,

$$U_p \cap V_q = \emptyset. \tag{5}$$

Indeed, if $p \neq q$ then, since X and Y form a k -pattern of $\text{FIX}(f)$, we have $x^p \leq y^q$ and $x^q \leq y^p$. Hence, if $v \in V_q$ then $x_v^q > y_v^q \geq x_v^p = 0$, so if $v \in U_p$ then $y_v^p = 0$ which implies $x_v^q = 0$, a contradiction. This proves (5).

As already said in Lemma 4, if $v \in V_p$, then $f_v(x^p) = x_v^p > y_v^p = f_v(y^p)$ and since f_v is monotone we deduce that G has an arc uv with $x_u^p > y_u^p$. Thus

$$G[V_p] \text{ has minimal in-degree at least one.} \tag{6}$$

Furthermore, if $v \in U_p \setminus V_p$, that is $x_v^p = y_v^p = \alpha$ for some $\alpha \in \{0, 1\}$, then $f_v(x^p) = f_v(y^p) = \alpha$. Hence, if f_v is not a constant then G has an arc uv with $u \in U_p$. Indeed, if $f_v \neq \text{cst}$ and $x_u^p < y_u^p$ for every arc uv of G , then $f_v(x^p) < f_v(y^p)$, a contradiction. We have thus the following property:

$$\text{If } v \in U_p \setminus V_p \text{ and } f_v \neq \text{cst} \text{ then } G \text{ has an arc } uv \text{ with } u \in U_p. \tag{7}$$

Let S^1, \dots, S^m be an enumeration of the strongly connected components of $G[U_p]$ in the topological order (that is, in such a way that $G[U_p]$ has no arcs from S^i to S^j if $j < i$). Let S^i be the first component containing a cycle. This component exists since, by property (6), $G[V_p]$ has a cycle and $V_p \subseteq U_p$. Suppose that $G[U_p]$ has an arc uv with $u \notin S^i$ and $v \in S^i$. Then $G[U_p]$ has a path P starting from an initial component S^j with $j < i$ and ending in u (initial means there are no arcs from S^ℓ to S^j for every $1 \leq \ell < j$). Then S_j has no cycles (since $j < i$) thus $S_j = \{w\}$ for some vertices w of in-degree zero in $G[U_p]$. We then deduce from (7) that $f_w = \text{cst}$, that is, w is a source of G . Thus P is a path from a source of G to u with only vertices in $U_p \setminus S^i$, and by adding the arc uv we obtain a path from a source to v with only internal vertices in $U_p \setminus S^i$. Setting $S_p = S^i$ we have thus the following property:

$$\text{If } G \text{ has an arc } uv \text{ with } v \in S_p \text{ and } u \in U_p \setminus S_p \text{ then } G \text{ has a path } P \text{ from a source of } G \text{ to } v \text{ with only internal vertices in } U_p \setminus S_p. \tag{8}$$

Since X_I and Y_I form a special k -pattern of L , we have $x_I^p = \overline{y_I^p}$ so that $U_p \cap I = V_p \cap I$. Hence $V_p \cap I$ is a feedback vertex set of $G[U_p]$ thus $S_p \cap V_p$ is not empty. According to (6) if $v \in S_p \cap V_p$

²If P has some internal vertices, and if none of them are in the packing then, obviously, no arcs of P is the packing. Thus the condition “ P has no arcs in the packing” makes sense only when P has no internal vertices, that is, when P is reduced to a single arc.

then either $G[V_p]$ has a cycle C containing v or $G[V_p]$ has a cycle C and a path from P from C to v . In both cases, by the choice of S_p , C is necessarily contained in $G[S_p]$. Thus

$$G[S_p \cap V_p] \text{ contains a cycle.}$$

For every $p \in [k]$, let C_p be a cycle of $G[S_p \cap V_p]$. From (5) these k cycles are mutually vertex-disjoint, so they form a packing, and it remains to prove that this packing is special. Suppose that G has a principal path P from C_p to C_q with $p \neq q$. Let v be the last vertex of P , and let u be the vertex preceding v in C_q . To complete the proof, we have to prove that G has a principal path from C_q to v or from a source of G to v . We consider two cases.

1. Suppose first that G has an arc wv such that $w \in U_q$ and $w \neq u$. If w is in C_q then the chord wv constitutes a principal path from C_q to v . If w is not in C_q and $w \in S_q$, then, since $G[S_q]$ is strongly connected, $G[S_q]$ has a path from C_q to w which, together with the arc wv , gives a principal path from C_q to v . If $w \notin S_q$ then, according to (8), G has a principal path from a source of G to v . This completes the first case.
2. Suppose now that v has no in-neighbors in U_q excepted u . Let w_1, \dots, w_r be an enumeration of the in-neighbors of v distinct from u , and let us right $f_v(z) = f_v(z_u, z_{w_1}, \dots, z_{w_r})$. We have $x_v^q > y_v^q$ and $x_u^q > y_u^q$ since $v, u \in V_q$. Also, for all $s \in [r]$, we have $x_{w_s}^q < y_{w_s}^q$ since $w_s \notin U_q$. Since f is monotone, we deduce that, for all $z_{w_1}, \dots, z_{w_r} \in \{0, 1\}$,

$$\begin{aligned} f_v(1, z_{w_1}, \dots, z_{w_r}) &\geq f_v(1, 0, \dots, 0) = f_v(x_u^q, x_{w_1}^q, \dots, x_{w_r}^q) = f_v(x^q) = x_v^q = 1 \\ f_v(0, z_{w_1}, \dots, z_{w_r}) &\leq f_v(0, 1, \dots, 1) = f_v(y_u^q, y_{w_1}^q, \dots, y_{w_r}^q) = f_v(y^q) = y_v^q = 0 \end{aligned}$$

Thus $f_v(z_u, z_{w_1}, \dots, z_{w_r}) = z_u$ for all $z_u, z_{w_1}, \dots, z_{w_r} \in \{0, 1\}$. It means that $f_v(z)$ only depends on z_u , so that u is the unique in-neighbor of v in G . Since u is in C_q , this contradict the existence of the principal path P from C_p to v . Thus the second case is actually not possible, and this completes the proof. □

Summarizing the previous results we get the following.

Theorem 2 (Upper bound for monotone Boolean networks). *If f is a monotone Boolean network with interaction graph G , then the set of fixed points of f is isomorphic to a subset $L \subseteq \{0, 1\}^\tau$ verifying the following conditions:*

1. L is a lattice,
2. L has no chains of size $\nu + 2$,
3. L has no $(\nu + 1)$ -patterns,
4. L has no special $(\nu^* + 1)$ -patterns.

Let us discuss some consequences of the fourth constraint, on special patterns and special packings. First, if $L = \{0, 1\}^\tau$ then L has a special τ -pattern and thus $\nu^* \geq \tau$, and since $\nu^* \leq \tau$ we get $\nu^* = \tau$. This shows that, for every digraph G ,

$$\phi_m(G) = 2^\tau \Rightarrow \nu^* = \tau. \tag{9}$$

In the next section, we will prove that the converse is true, thus showing that the notions of special pattern and special packing are very natural in our context.

We can actually prove a more general implication. Let x^- and x^+ be the minimal and maximal element of L , and let $L' = L \setminus \{x^-, x^+\}$. Since L' has no chains of size ν , as mentioned above, it results from a theorem of Erdős [6] that $|L'|$ is at most the sum of the $\nu - 1$ largest binomial coefficients $\binom{\tau}{k}$. Suppose that $|L'|$ reaches this sum, and let $\ell = \frac{\tau - \nu + 2}{2}$. Erdős, Füredi and Katona [7] proved that L' is then the union of the set $\binom{[\tau]}{k}$ where k ranges either in the interval $[[\ell], \lfloor \tau - \ell \rfloor]$ or in the interval $[[\ell], \lceil \tau - \ell \rceil]$. In both cases, $\binom{[\tau]}{[\ell]}$ and $\binom{[\tau]}{\tau - \lceil \ell \rceil}$ are contained in L' so, by (3), L' has a special $\lfloor \frac{\tau}{\lceil \ell \rceil} \rfloor$ -pattern. As a consequence of the fourth constraint we get $\nu^* \geq \lfloor \frac{\tau}{\lceil \ell \rceil} \rfloor$. This shows that, for all digraph G ,

$$\phi_m(G) = 2 + \sum_{k=\lfloor \frac{\tau - \nu + 2}{2} \rfloor}^{\lfloor \frac{\tau + \nu - 2}{2} \rfloor} \binom{\tau}{k} \Rightarrow \nu^* \geq \left\lfloor \frac{\tau}{\lceil \frac{\tau - \nu + 2}{2} \rceil} \right\rfloor$$

In particular, if $\phi_m(G) = 2^\tau$ then $\nu = \tau$ and we deduce that $\nu^* = \tau$. We thus recover (9).

It is important to note that, contrary to ν , for a fixed ν^* the transversal number τ can be arbitrarily large. For instance, if T'_n denotes the digraph obtained from the transitive tournament on n vertices by adding a loop on each vertex, then we have $\nu^*(T'_n) = 1$ and $\nu(T'_n) = \tau(T'_n) = n$. In the next section we will exhibit a family of strongly connected digraphs with a similar property (cf. Proposition 2). Thus bounding ν^* is much more weaker than bounding ν , and considering the case $\nu^* = 1$ could be interesting.

So suppose that $\nu^* = 1$. According to the fourth constraints, L has no special 2-patterns, and thus L' has no special 2-patterns. Hence, by (4), this is equivalent to say that $L' \cap \overline{L'} = \emptyset$. Let t be the number of $v \in [\tau]$ such that $x_v^- < x_v^+$, and let X be the set of $x \in \{0, 1\}^\tau$ such that $x^- < x < x^+$. Then $L' \subseteq X$ and X is isomorphic to $\{0, 1\}^t \setminus \{0, 1\}$. Since $L' \cap \overline{L'} = \emptyset$ we deduce that $|L'| \leq \frac{2^t - 2}{2} \leq 2^{\tau-1} - 1$ so that $|L| \leq 2^{\tau-1} + 1$. Thus, for every digraph G ,

$$\nu^* = 1 \Rightarrow \phi_m(G) \leq 2^{\tau-1} + 1.$$

3 Lower bound for monotone networks

3.1 Optimal linear lower bound in ν

Lemma 6. *For every digraph G ,*

$$\nu + 1 \leq \phi_m(G).$$

Proof. Suppose that G has vertex set $[n]$. Let C_1, \dots, C_ν be vertex-disjoint cycles in G , and for every $p \in [\nu]$, let V_p be the vertices of C_p . Let U_0 be the set of vertices that cannot be reached from one of these cycles (U_0 may be empty). Let U_1 be the set of vertices reachable from C_1 in $G \setminus (V_2 \cup \dots \cup V_\nu)$. For $2 \leq p \leq \nu$, let U_p be the set of vertices reachable from C_p in $G \setminus (U_1 \cup \dots \cup U_{p-1} \cup V_{p+1} \cup \dots \cup V_\nu)$. In this way $\{U_0, U_1, \dots, U_\nu\}$ is a partition of the vertex set of G . Note that every $G[U_p]$ is of minimal in-degree at least one.

For every $0 \leq p \leq \nu$ and every $v \in U_p$ we set

$$\theta_v = |N_G^-(v) \cap (U_0 \cup \dots \cup U_p)|.$$

Let $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ be defined for every $v \in [n]$ by:

$$f_v(x) = \begin{cases} 1 & \text{if } \sum_{u \in N_G^-(v)} x_u \geq \theta_v. \\ 0 & \text{otherwise.} \end{cases}$$

It is easy to check that f is monotone and that G is its interaction graph. For $1 \leq q \leq \nu$, let $x^q \in \{0, 1\}^n$ be defined for every $v \in [n]$ by:

$$x_v^q = \begin{cases} 1 & \text{if } v \in U_0 \cup \dots \cup U_q \\ 0 & \text{otherwise.} \end{cases}$$

We claim that each x^q is a fixed point of f . So let $q \in [\nu]$ and let $v \in U_p$ with $0 \leq p \leq \nu$. Then

$$\sum_{u \in N_G^-(v)} x_u^q = |N_G^-(v) \cap (U_0 \cup \dots \cup U_q)|.$$

Hence if $0 \leq p \leq q$ this sum is at least θ_v , and thus $f_v(x^q) = 1 = x_v^q$. If $q < p$ then this sum is at most $\theta_v - 1$, because $N_G^-(v) \cap U_p \neq \emptyset$ (by construction $G[U_p]$ is of minimal-indegree at least one), and we deduce that $f_v(x^q) = 0 = x_v^q$. Thus x^1, \dots, x^ν are distinct fixed points of f , and since $f(0) = 0$ this completes the proof. \square

We will now prove that this lower bound is tight. For that we first identify a rather general class of networks without $\nu + 2$ fixed points. Let $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ be a Boolean network with interaction graph G . We say that f is an *and-or-network* if for every $v \in [n]$ we have either $f_v(x) = \bigwedge_{u \in N_G^-(v)} x_u$ for all $x \in \{0, 1\}^n$ or $f_v(x) = \bigvee_{u \in N_G^-(v)} x_u$ for all $x \in \{0, 1\}^n$ (by convention, the empty conjunction is 1 and the empty disjunction is 0). In the first case we say that v is an *and-vertex* and in the second case we say that v is an *or-vertex*. We say that two vertex-disjoint cycle C_1 and C_2 of G are *independent* if G has no arcs from C_1 to C_2 and no arcs from C_2 to C_1 .

Lemma 7. *Let f be an and-or-network with interaction graph G . If G has no two independent cycles, then f has at most $\nu + 1$ fixed points.*

Proof. Suppose that x^1 and x^2 be two fixed points of f . Let I^1 be the set of vertices v such that $x_v^1 > x_v^2$, and let I^2 be the set of vertices v such that $x_v^2 > x_v^1$. Suppose that x^1 and x^2 are incomparable. Then both I^1 and I^2 are not empty and it is easy to check that both $G[I_1]$ and $G[I_2]$ are of minimal in-degree at least one. Thus $G[I_1]$ contains a cycle C_1 and $G[I_2]$ contains a cycle C_2 . Furthermore, there is no arc uv with $u \in I_1$ and $v \in I_2$. Suppose indeed that such an arc uv exists. Since $x_u^1 = 1$ and $x_v^1 = 0 = f_v(x^1)$, v cannot be an or-vertex, and since $x_u^2 = 0$ and $x_v^2 = 1 = f_v(x^2)$, v cannot be an and-vertex, a contradiction. Thus there are no arcs from I_1 to I_2 and by symmetry there are no arcs from I_2 to I_1 . Thus C_1 and C_2 are two independent cycles of G . We have thus prove the following: *If f has two incomparable fixed points then G has two independent cycles.* Therefore, if G has no two independent cycles then $\text{FIX}(f)$ is a chain, which is, by Lemma 3, of size at most $\nu + 1$. \square

Lemma 8. *If G is a digraph with maximal in-degree ≤ 2 and with no two independent cycles, then $\phi_m(G) = \nu + 1$.*

Proof. This results from Lemma 6, Lemma 7 and the following basic observation: if G is of maximal in-degree at most two then every monotone Boolean network with G has interaction graph is an and-or-network. \square

Let us now exhibit, for every k , a strongly connected digraph G verifying the conditions of the previous lemma and such that $\nu = k$. For every $n \geq 1$, let K_n^* be the directed graph defined as follows. The set of vertices is $N \times N$, with $N = \{0, 1, \dots, n-1\}$, and the set of arcs is defined as follows, where sums are computed modulo n :

1. for all $i, j \in N$, there is an arc from (i, j) to $(i, j + 1)$.
2. for all $i, j \in N$ with $i \neq j$, there is an arc from (i, i) to (j, i) .

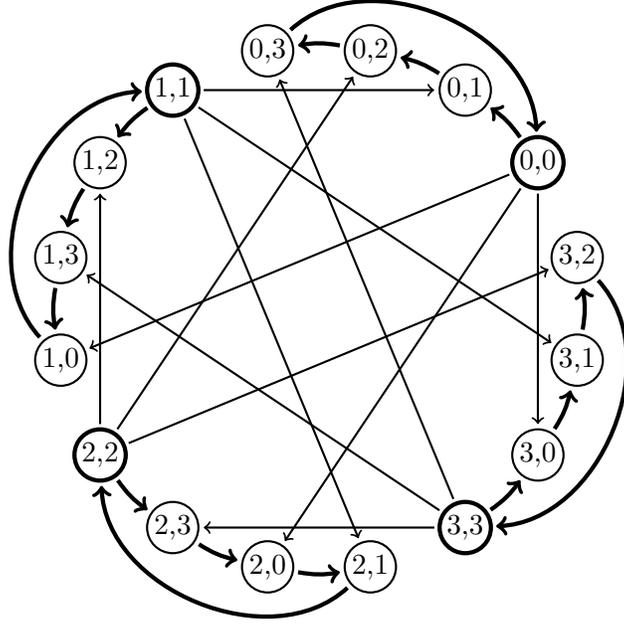


Figure 3: K_4^* .

Proposition 2. *For all $n \geq 1$, we have $\nu(K_n^*) = \tau(K_n^*) = n$ and $\nu^*(K_n^*) = 1$. Furthermore, K_n^* has maximal in-degree at most two and no two independent cycles, so that $\phi_m(K_n^*) = n + 1$.*

Proof. Foremost, each vertex (i, j) of K_n^* with $i \neq j$ has exactly two in-neighbors, namely $(i, j - 1)$ and (j, j) (sums and differences are computed modulo n). Also, each vertex (i, i) has a unique in-neighbor, namely $(i, i - 1)$. Thus K_n^* has maximal in-degree at most two.

For each $i \in N$, the set of vertices $\{i\} \times N$ induces a cycle of length n , denoted C_i . These cycles C_i are obviously pairwise vertex-disjoint, thus $\nu(K_n^*) \geq n$. Furthermore, since each vertex of C_i distinct from (i, i) has a unique out-neighbor, we deduce that every cycle C meeting C_i contains the vertex (i, i) . We deduce that the set of vertices $I = \{(i, i) \mid i \in N\}$ is a feedback vertex set. Thus $\tau(K_n^*) = n$, and we deduce that $\nu(K_n^*) = n$.

We will prove that K_n^* has no two independent cycles. Let F_1 and F_2 be two vertex-disjoint cycles of K_n^* . Suppose, for a contradiction, that F_1 and F_2 are independent. Let $(i_1, i_1) \in F_1 \cap I$ and $(i_2, i_2) \in F_2 \cap I$ be such that $|i_1 - i_2|$ is minimal. Without loss of generality, we can suppose that $i_2 < i_1$. Since there is an arc from (i_2, i_2) to (i_1, i_2) , (i_1, i_2) is not a vertex of F_1 , thus $F_1 \neq C_{i_1}$ and we deduce that F_1 contains an arc of the form a vertex (j, j) to (i_1, j) , with $j \neq i_1, i_2$. Let P be the path from (i_1, j) to (i_1, i_1) contained in C_{i_1} . Clearly, this path P is also contained in F_1 . Thus, if $0 \leq j < i_2$ or $i_1 < j \leq n - 1$, then (i_1, i_2) is a vertex of P , a contradiction. We deduce that $i_2 < j < i_1$. Thus $|j - i_2| < |i_1 - i_2|$ and since $(j, j) \in F_1 \cap I$, this contradicts our choice of (i_1, i_1) and (i_2, i_2) . We deduce that K_n^* has no two independent cycles. Thus, by Lemma 8, $\phi_m(K_n^*) = \nu + 1$.

Let us now prove that $\nu^* = 1$. Let F_1 and F_2 be two vertex-disjoint cycles. Since they are not independent, there exists an arc uv between the two cycles, say from F_1 to F_2 . This arc then constitutes a principal path from F_1 to F_2 . Since v is of in-degree exactly 2, every principal path ending in v contains uv . Thus uv is actually the unique principal path ending in v , and thus $\{F_1, F_2\}$ cannot be a special packing. \square

3.2 Optimal exponential lower bound in ν^*

Lemma 9. *For every digraph G ,*

$$2^{\nu^*} \leq \phi_m(G).$$

More precisely, there exists a monotone Boolean network f with G as interaction graph such that f has at least 2^{ν^} fixed points and $f_v = \text{cst} = 0$ for every source v of G .*

Proof. Suppose that G has vertex set $V = [n]$. Let \mathcal{P} be a special packing of size ν^* . Let U be the set of vertices that belong to some cycle of the packing, and let S be the set of sources of G . Every $v \in U$ has exactly one in-neighbor that belongs to the same cycle than v of the packing. We denote it v' . Let $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ be defined by

$$\begin{aligned} f_v(x) &= x_{v'} \vee \bigwedge_{u \in N_G^-(v) \setminus \{v'\}} x_u & \forall v \in U \\ f_v(x) &= 0 & \forall v \in S \\ f_v(x) &= \bigwedge_{u \in N_G^-(v)} x_u & \forall v \in V \setminus (U \cup S). \end{aligned}$$

Clearly, f is monotone and its interaction graph is G .

Let $\mathcal{I} \subseteq \mathcal{P}$ be a subset of cycles in the packing and let I be the set of vertices that belongs to a cycle of \mathcal{I} . Let $J = \{v_1, v_2, \dots, v_r\}$ be a maximal sequence of vertices in $V \setminus I$ such that $N_G^-(v_1) \subseteq I$ and $N_G^-(v_i) \subseteq I \cup \{v_1, \dots, v_{i-1}\}$ for all $1 < i \leq r$ (J may be empty). By construction, $G[J]$ intersect no cycle of G disjoint from I , so that $J \cap U = \emptyset$. Let us defined $x^{\mathcal{I}} \in \{0, 1\}^n$ by

$$x_v^{\mathcal{I}} = \begin{cases} 1 & \text{if } v \in I \cup J \\ 0 & \text{otherwise.} \end{cases}$$

Suppose that $\mathcal{I}' \subseteq \mathcal{P}$ and $\mathcal{I}' \neq \mathcal{I}$. If C is a cycle of $\mathcal{I}' \setminus \mathcal{I}$ and v is a vertex of C then $v \in U \setminus I$ and since $J \cap U = \emptyset$ we have $x_v^{\mathcal{I}} = 0$. Since $x_v^{\mathcal{I}'} = 1$, this show that $x^{\mathcal{I}} \neq x^{\mathcal{I}'}$, and if $\mathcal{I}' \setminus \mathcal{I} \neq \emptyset$ we obtained the same conclusion with similar arguments. Thus the 2^{ν^*} possible choices of \mathcal{I} gives 2^{ν^*} distinct points $x^{\mathcal{I}}$. It is thus sufficient to prove that $x^{\mathcal{I}}$ is a fixed point.

To simplify notations we set $x = x^{\mathcal{I}}$. First, for all $v \in I$ we have $x_{v'} = 1$ and thus $f_v(x) = 1 = x_v$. Then, with a straightforward induction on $i = 1, \dots, r$, we prove that $f_{v_i}(x) = 1 = x_{v_i}$. Consequently, $f_v(x) = 1 = x_v$ for all $v \in I \cup J$. Furthermore, if $v \in S$ then $f_v(x) = 0$ by definition, so $v \notin I \cup J$ and thus $f_v(x) = 0 = x_v$. Next, let $v \in V \setminus (U \cup J \cup S)$. If $f_v(x) = 1$, then $N_G^-(v) \subseteq I \cup J$ and this contradicts the maximality of J , thus $f_v(x) = 0 = x_v$. Finally, suppose that $v \in U \setminus I$, so that $x_v = 0$, and let C be the cycle of \mathcal{P} containing v . If $N_G^-(v) \cap (I \cup J) = \emptyset$, then $f_v(x) = 0 = x_v$. So suppose that there exists $u \in N_G^-(v) \cap (I \cup J)$. Then there exists a shortest path from I to u with only vertices in $I \cup J$, and with the arc uv this gives a principal path P from a cycle of \mathcal{I} to v . Since \mathcal{P} is a special packing, there exists another principal path $P = u_1, \dots, u_p, v$ such that either u_1 is a source or u_1 belongs to C . In both cases, $x_{u_1} = 0$, and since the internal vertices u_i , $1 < i \leq p$, are not in $U \cup S$, we deduce, by induction on i , that $f_{u_i}(x) = 0 = x_{u_i}$. Thus $x_{u_p} = 0$ and since $u_p \neq v'$ we have $f_v(x) = 0 = x_v$. \square

The lower bound 2^{ν^*} gives the other direction of the implication (9) and we thus get the following characterization.

Theorem 3. *For every digraph G ,*

$$\phi_m(G) = 2^\tau \iff \nu^* = \tau.$$

The most simple example of digraph such that $\nu^* = \tau$ is the union of k disjoint cycles. See Figures 2 for families of strongly connected digraphs with this property.

3.3 Introduction of the circumference in the lower bound

In this section, we prove that if a digraph G has many vertex-disjoint *short* cycles, then we can construct a monotone Boolean network with interaction graph G and with many fixed points.

For that we use the lower bound 2^{ν^*} and a result about domination in digraphs. In a digraph $G = (V, A)$, a *dominating set* is a set of vertices $D \subseteq V$ such that every vertex in $V \setminus D$ has an in-neighbor in D . Using probabilistic arguments, Lee [18] proved the following result: *If G has minimal in-degree at least one, then G has a dominating set of size at most $3|V|/2$.* We use this result to prove the next lemma, which is actually a generalization (we recover the result of Lee by taking $U = V$, $|V| = k$, $\ell = 1$, and by assuming that G has minimal in-degree at least one).

Lemma 10. *Let G be a digraph, let U be non-empty subset of vertices of G and let (U_1, \dots, U_k) be a partition of U . For every $i \in [k]$, let U'_i be a non-empty subset of U_i of size at most ℓ . Then there exists a subset $I \subseteq [k]$ of size at least $k/3^\ell$ such that for every $i \in I$ and every $u \in U'_i$ one of the following condition holds:*

1. G has a path from $U \setminus \bigcup_{j \in I} U_j$ to u without internal vertex in U .
2. G has no path from $U \setminus U_i$ to u .

Proof. We proceed by induction on ℓ assuming that $\ell = \max_{i \in [k]} |U'_i|$.

If $\ell = 1$ then for every $i \in [k]$ there exists $u_i \in U_i$ such that $U'_i = \{u_i\}$. Let H be the digraph on $[k]$ with an arc ij if and only if $i \neq j$ and G has a path from U_i to u_j without internal vertex in U . Let S be the set of $i \in [k]$ such that u_i is a source of H . If $|S| \geq k/3$ then $I = S$ has the desired properties. So suppose that $|S| < k/3$. Let H' be obtained from H by adding an arc ij for every $j \in S$ and $i \in [k] \setminus S$. In this way, the minimal in-degree of H' is at least one. Consequently, by the result of Lee [18] mentioned above, H' has a dominating set D of size at most $2k/3$. Thus $I = [k] \setminus D$ is of size at most $k/3$. Furthermore, by construction: for every $i \in I \setminus S$, there exists $j \in D$ such that G has a path from U_j to u_i without internal vertex in U ; and for every $i \in I \cap S$, G has no path from $U \setminus U_i$ to u_i . Thus I has the desired properties. This prove the case $\ell = 1$.

Now suppose that $\ell \geq 2$ and for every $i \in [k]$, let $u_i \in U'_i$. According to the case $\ell = 1$ there exists a subset $I \subseteq [k]$ of size at least $k/3$ such that:

$$\text{For every } i \in I, \text{ either } G \text{ has a path from } U \setminus \bigcup_{j \in I} U_j \text{ to } u_i \text{ without} \\ \text{internal vertex in } U, \text{ or } G \text{ has no path from } U \setminus U_i \text{ to } u_i. \quad (10)$$

Now, for every $i \in I$ we set $U''_i = U'_i$ if $U'_i = \{u_i\}$ and $U''_i = U'_i - \{u_i\}$ otherwise. Then $\max_{i \in [k]} |U''_i| = \ell - 1$. Hence, by induction hypothesis, there exists a subset $I' \subseteq I$ of size at least $|I|/3^{\ell-1}$ such that:

$$\text{For every } i \in I' \text{ and every } u \in U''_i, \text{ either } G \text{ has a path from } U \setminus \bigcup_{j \in I'} U_j \\ \text{to } u \text{ without internal vertex in } U, \text{ or } G \text{ has no path from } U \setminus U_i \text{ to } u. \quad (11)$$

So $|I'| \geq |I|/3^{\ell-1} \geq k/3^\ell$ and we deduce from (10) and (11) that I' has the desired properties. \square

We are now in position to prove the following lower bound, using the preceding lemma and the lower bound 2^{ν^*} .

Lemma 11. *If a digraph G has k disjoint cycles of length at most ℓ then*

$$2^{k/3^\ell} \leq \phi_m(G).$$

Proof. Suppose that G has vertex set $[n]$ and let C_1, \dots, C_k be disjoint cycles of G of length at most ℓ . For all $i \in [k]$, let U_i be the set of vertices of C_i , and let $U = U_1 \cup \dots \cup U_k$. According to Lemma 10, there exists a subset $I \subseteq [k]$ of size at least $k/3^\ell$ such that for every $i \in I$ and every $u \in U_i$, either G has a path from $U \setminus \bigcup_{j \in I} U_j$ to u without internal vertex in U , or G has no path from $U \setminus U_i$ to u .

Let $W = U \setminus \bigcup_{i \in I} U_i$ and let G' be obtained from G by removing every arc vw with $w \in W$. and let us prove that $\mathcal{P} = \{C_i : i \in I\}$ is a special packing of G' . So let $i \in I$, $u \in U_i$ and suppose that G' has a principal path P from a cycle $C_j \neq C_i$ to u . Then G has a path from $U \setminus U_i$ to U_i , and we deduce that G has a path from W to u without internal vertices in U , and since every vertex of W is a source of G' , we deduce that G' has a principal path from a source to u . Thus \mathcal{P} is indeed a special packing of G' of size $|I|$. Thus according to Lemma 9 there exists a monotone Boolean network f' with interaction graph G' such that f' has at least $2^{|I|}$ fixed points and $f' = \text{cst} = 0$ for every source v of G' .

Let $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ be the Boolean network defined for all $v \in [n]$ by,

$$f_v(x) = \begin{cases} f'_v(x) & \text{if } v \notin W \\ \bigwedge_{u \in N_G^-(v)} x_u & \text{otherwise.} \end{cases}$$

Then f is monotone and G is the interaction graph of f . Furthermore, if x is a fixed point of f' then $f_v(x) = f'_v(x) = x_v$ for all $v \notin W$ and $x_W = 0$. Since if $v \in W$ then $N_G^-(v) \cap W \neq \emptyset$ we deduce that $f_v(x) = 0 = x_v$. Thus x is a fixed point of f . Thus f has at least as many fixed points as f' and this completes the proof. \square

The *circumference* $c = c(G)$ of a digraph G is the maximal length of a chordless cycle of G . Since every digraph G has always a packing of ν chordless cycles, we deduce from the preceding lemma that $2^{\nu/3^c} \leq \phi_m(G)$. Furthermore, the set of vertices that belongs to packing of ν chordless cycles is always a feedback vertex set. Thus we always have $\tau \leq c\nu$ and has a consequence, for every digraph G ,

$$2^{\nu/3^c} \leq \phi_m(G) \leq 2^{c\nu}.$$

This lower bound can be much more better than the two previous one. As an example, for the transitive tournament on n vertices with loop on each vertex we have $\nu^* = c = 1$ and $\nu = n$.

Summarizing the previous results we get the following.

Theorem 4 (Lower bounds for monotone Boolean networks). *For every digraph G ,*

$$\max(\nu + 1, 2^{\nu^*}, 2^{\nu/3^c}) \leq \phi_m(G).$$

3.4 The undirected case

We say that a digraph G is *symmetric* if, for every distinct vertices u and v , either uv and vu are not arcs, or both uv and vu are arcs. Hence, a loop-less symmetric digraph G can be seen as a simple *undirected* graph, simply by seeing every 2-cycle (cycle of length two) as an undirected edge. Since a loop-less symmetric digraph G has circumference $c = 2$ we have $2^{\nu/9} \leq \phi_m(G)$ and this contrasts with the general case where the tight linear lower bound $\nu + 1$ holds. Below, we prove something stronger: we prove that $\nu/6 \leq \nu^*$, from which we immediately get $2^{\nu/6} \leq \phi_m(G)$. This connection between ν and ν^* also contrasts with the general case, where we can have $\nu^* = 1$ and ν arbitrarily large (cf. Proposition 2).

Proposition 3. *For every loop-less symmetric digraph G ,*

$$\nu/6 \leq \nu^* \leq \nu \leq \tau \leq 2\nu.$$

Proof. The inequality $\tau \leq 2\nu$ comes from the fact that the circumference of G is $c = 2$, so the only thing to prove is $\nu/6 \leq \nu^*$. Below, we see G has an simple undirected graph, that is, we see a cycle of length two between two vertices u and v has an undirected edge uv . If uv is an edge, we say that u and v are *adjacent*, and we say that a vertex w *covers* uv if $w = u$ or $w = v$. A *matching* is a set of vertex-disjoint edges. Clearly, ν is the maximum size of a matching in G . We say a vertex belongs to a matching M is it covers one of the edges of M .

Suppose that G has a matching M satisfying the following property:

If G has an edge uv where u and v covers different edges of the matching, then v is adjacent to some vertex that does not belong to the matching. (*)

We claim that M is then a *special matching* (that is, the cycles of length two corresponding to the edges of M form a special packing). Indeed, suppose that $M = \{u_1v_1, \dots, u_kv_k\}$ and suppose that G has a principal path P from $u \in \{u_i, v_i\}$ to $v \in \{u_j, v_j\}$ for some distinct $i, j \in [k]$. If P is of length at least two, then the vertex w preceding v in P is not in the matching, and $P' = vvw$ is a principal path from $\{u_j, v_j\}$ to v . If P is of length one, then P is reduced to the arc uv and we deduce from the property (*) that v is adjacent to a vertex w that is not in the matching, and thus, as previously, $P' = vvw$ is a principal path from $\{u_j, v_j\}$ to v . Thus M is indeed a special matching. Therefore, to prove the proposition it is sufficient to prove G has a matching of size at least $\nu/6$ with the property (*).

Let $M_1 = \{u_1v_1, \dots, u_\nu v_\nu\}$ be a matching of size ν , and let G_1 be the simple undirected graph whose vertices are the edges of M_1 and with an edge between u_iv_i and u_jv_j if G has an edge uv with $u \in \{u_i, v_i\}$ and $v \in \{u_j, v_j\}$. Let I_1 be the set of isolated vertices of G_1 . Hence, in G , we have the following property:

For every $u_iv_i \in I_1$, u_i and v_i are adjacent to no vertices in $M_1 \setminus \{u_iv_i\}$. (12)

Now, since $G_1 \setminus I_1$ has no isolated vertices, it contains an dominating set D_1 of size at most $(\nu - |I_1|)/2$ (this is a basic result about domination in graphs, see for instance [13, Theorem 2.1]). Thus the complement $M_2 = M_1 \setminus (I_1 \cup D_1)$ has size at least $(\nu - |I_1|)/2$. Hence, by construction, in G , for every edge $u_iv_i \in M_2$, u_i or v_i (or both) is adjacent to some vertex that belongs to the matching D_1 . So without loss of generality, we can suppose that G has the following property:

For every $u_iv_i \in M_2$, v_i is adjacent to some vertex in D_1 . (13)

Let G_2 be the *digraph* whose the vertices are the edges of the matching M_2 and with an arc directed from u_iv_i to u_jv_j if G has an edge uv with $u \in \{u_i, v_i\}$ and $v \in \{u_j, v_j\}$. Let I_2 be the set vertices of in-degree zero in G_2 . Hence, in G , we have the following property:

For every $u_iv_i \in I_2$, u_i is adjacent to no vertices in $M_2 \setminus \{u_iv_i\}$. (14)

Let \tilde{G}_2 be obtained from G_2 by adding an arc from every $u_iv_i \in M_2$ to every $u_jv_j \in I_2$, with $i \neq j$. Since \tilde{G}_2 has minimal in-degree at least one, by the result of Lee [18] mentioned above, it has a dominating set D_2 of size at most $3|M_2|/2$. Thus the complement $M_3 = M_2 \setminus D_2$ has size at least $|M_2|/3$. Hence, by construction, in G we have the following property:

For every $u_iv_i \in M_3 \setminus I_2$, u_i is adjacent to some vertex in D_2 . (15)

We have

$$|M_3| \geq \frac{|M_2|}{3} \geq \frac{\nu - |I_1|}{6} \geq \frac{\nu}{6} - |I_1|,$$

thus it is sufficient to prove that $I_1 \cup M_3$ has the property (*). Suppose that G has an edge uv where u and v cover different edges of $I_1 \cup M_3$, say $u_i v_i$ and $u_j v_j$ respectively. Then, according to (12), $u_i v_i$ and $u_j v_j$ are not in I_1 , and thus they belong to M_3 . Furthermore, if $v = v_j$ then since $M_3 \subseteq M_2$ we deduce from (13) that v is adjacent to some vertices that is not $I_1 \cup M_3$. If $v = u_j$ then we deduce from (14) that $u_j v_j \notin I_2$. Hence, according to (15), we deduce that $v = u_j$ is adjacent to some vertex not in $I_1 \cup M_3$. Thus, in every case, v is adjacent to some vertex not in $I_1 \cup M_3$. We prove with similar arguments that u is adjacent to some vertex not in $I_1 \cup M_3$. Thus $I_1 \cup M_3$ has the property (*) and this completes the proof. \square

4 Upper bound for signed digraphs

A *signed digraph* is a couple (G, σ) where G is a digraph and σ is an arc-labeling function taking its values in $\{-1, 0, 1\}$. An *undirected cycle* is a sequence of distinct vertices v_0, \dots, v_ℓ such that G has an arc from v_k to v_{k+1} or from v_{k+1} to v_k for all $0 \leq k \leq \ell$ (where $k+1$ is computed modulo $\ell+1$). The sign of a (directed or undirected) cycle is the product of the signs of its arcs. We say that (G, σ) is *balanced* when all its directed and undirected cycles are positive. The notion of balance is central in the study of signed digraphs [12, 30, 31].

The *signed interaction graph* of a Boolean network $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ is the signed digraph (G, σ) where G is the interaction graph of f and where σ is the arc-labeling function defined for all arc uv of G by

$$\sigma(uv) = \begin{cases} 1 & \text{if } f_v(x) \leq f_v(x + e_u) \text{ for all } x \in \{0, 1\}^n \text{ with } x_u = 0, \\ -1 & \text{if } f_v(x) \geq f_v(x + e_u) \text{ for all } x \in \{0, 1\}^n \text{ with } x_u = 0, \\ 0 & \text{otherwise.} \end{cases}$$

Given a digraph (G, σ) , we denote by $\phi(G, \sigma)$ the maximum number of fixed points in a Boolean network whose signed interaction graph is (isomorphic to) (G, σ) . Furthermore, we denote by $\tau^+ = \tau^+(G, \sigma)$ the minimum size of a set of vertices intersecting every *non-negative* cycle, and we denote by ν^+ the maximum number of vertex-disjoint *non-negative* cycles of (G, σ) . We have, obviously, $\nu^+ \leq \tau^+ \leq \tau$ and $\nu^+ \leq \nu$. One of the authors [3] proved the following generalization of the classical upper bound 2^τ : for every signed digraph (G, σ) ,

$$\phi(G, \sigma) \leq 2^{\tau^+}.$$

In this section, discuss previous results on monotone networks in the context of signed digraphs, and we will establish an upper bound, competitive with 2^{τ^+} , which is also based on the cycle structure. Let us start with a basic observation. Given a Boolean network f with signed interaction graph (G, σ) , and a vertex v in this graph, it is easy to see that f_v is monotone if and only if $\sigma(uv) = 1$ for every in-neighbor u of v . As a consequence, f is monotone if and only if $\sigma = \text{cst} = 1$, and we deduce that

$$\sigma = \text{cst} = 1 \Rightarrow \phi(G, \sigma) = \phi_m(G). \quad (16)$$

To go further we need an usual operation on signed digraphs, called *switch* [30]. Given a signed digraph (G, σ) and a subset I of vertices of G , the *I-switch* of (G, σ) is the signed digraph (G, σ^I) where σ^I is defined for every arc uv of G by

$$\sigma^I(uv) = \begin{cases} \sigma(uv) & \text{if } u, v \in I \text{ or } u, v \notin I, \\ -\sigma(uv) & \text{otherwise.} \end{cases}$$

Observe that every cycle C of G has the same sign in (G, σ) and (G, σ^I) . As a consequence ν^+ and τ^+ are invariant under the switch operation. Below, we prove that ϕ is also invariant under the switch operation.

Lemma 12. *Let (G, σ) be a signed digraph and let I be a subset of its vertices. Then*

$$\phi(G, \sigma) = \phi(G, \sigma^I).$$

Proof. Let $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$ be a Boolean network with (G, σ) as signed interaction graph and with $\phi(G, \sigma)$ fixed points. Let $f^I : \{0, 1\}^n \rightarrow \{0, 1\}^n$ be defined by

$$f^I(x) = f(x + e_I) + e_I.$$

It is easy to check that $f(x) = x$ if and only if $f^I(x + e_I) = x + e_I$. Thus f and f^I have the same number of fixed points. It is also easy to check that (G, σ^I) is the signed interaction graph of f^I . Hence, $\phi(G, \sigma) \leq \phi(G, \sigma^I)$ so that $\phi(G, \sigma^I) \leq \phi(G, (\sigma^I)^I)$. Since $(\sigma^I)^I = \sigma$ we have $\phi(G, \sigma^I) \leq \phi(G, \sigma)$ and this completes the proof. \square

Given a signed digraph (G, σ) , the *frustration index* (sometime called *index of imbalance*), denoted $\lambda = \lambda(G, \sigma)$, is the minimum number of non-positive arcs in a switch of (G, σ) . A basic result in signed graph theory is that λ can be equivalently defined as the minimum number of arcs whose deletion in (G, σ) yield a balanced signed digraph [12]. Hence, the following assertions are equivalent: $\lambda = 0$; (G, σ) is balanced; there exists a subset of vertices I such that $\sigma^I = \text{cst} = 1$. We then deduce from (16) and Lemma 12 that, for every signed digraph (G, σ) ,

$$[(G, \sigma) \text{ is balanced} \iff \lambda = 0] \implies \phi(G, \sigma) = \phi_m(G).$$

We now introduced an upper bound on $\phi(G, \sigma)$ that is competitive with 2^{τ^+} . A *monotone feedback vertex set* in signed digraph (G, σ) is a feedback vertex I of G such that $\sigma(uv) = 1$ for every arc uv of G with $v \notin I$. We denote by $\tau_m = \tau_m(G, \sigma)$ the minimum size of a monotone feedback vertex set of (G, σ) . We have, obviously, $\tau \leq \tau_m$. As an immediate application of two lemmas introduced to bound $\phi_m(G)$ we have the following property.

Lemma 13. *Let f be a Boolean network with signed interaction graph (G, σ) . The number of fixed points in f is at most the sum of the $\nu^+ + 1$ largest binomial coefficients $\binom{\tau_m}{k}$.*

Proof. Let I be a monotone feedback vertex set of (G, σ) of size τ_m . If $v \notin I$ then $\sigma(uv) = 1$ for all $u \in N_G^-(v)$, so that f_v is monotone. Hence, by Lemma 2, $\text{FIX}(f)$ is isomorphic to a subset $X \subseteq \{0, 1\}^I$, and by Lemma 3, X has no chains of size $\nu^+ + 2$. Hence, by the Erdős' theorem already used in the proof of Theorem 1, we deduce that $|X|$ is at most the sum of the $\nu^+ + 1$ largest binomial coefficients $\binom{I}{k}$. \square

Contrary to ν^+ , τ^+ , λ and ϕ , the parameter τ_m is not invariant under the switch operation. Consider for instance the loop-less symmetric digraph $K_{n,n}$ corresponding to the complete bipartite graph with both parts of size n . Let $K_{n,n}^+$ (resp. $K_{n,n}^-$) be the signed digraphs obtained from $K_{n,n}$ by labeling every arc positively (resp. negatively). We have $\tau_m(K_{n,n}^-) = 2n$ and $\tau_m(K_{n,n}^+) = \tau(K_{n,n}) = n$. Furthermore, $K_{n,n}^+$ is the switch of $K_{n,n}^-$ by one of the two parts. Thus, given a signed digraph (G, σ) with vertex set V , it makes sense consider the parameter $\tilde{\tau}_m$ defined as the minimum size of a monotone feedback vertex set in a switch of (G, σ) , that is,

$$\tilde{\tau}_m = \tilde{\tau}_m(G, \sigma) = \min_{I \subseteq V} \tau_m(G, \sigma^I).$$

Graph parameters based on feedback vertex sets are thus ordered as follows:

$$\tau^+ \leq \tau \leq \tilde{\tau}_m \leq \tau_m$$

We have now the following upper bound that improved the one of Lemma 13.

Theorem 5. *Let f be Boolean network with signed interaction graph (G, σ) . The number of fixed points in f is at most the sum of the $\nu^+ + 1$ largest binomial coefficients $\binom{\tilde{\tau}_m}{k}$.*

Proof. Let I be such that $\tilde{\tau}_m = \tilde{\tau}_m(G, \sigma) = \tau_m(G, \sigma^I)$. According to Lemma 13, $\phi(G, \sigma^I)$ is at most the sum of the $\nu^+(G, \sigma^I) + 1$ largest binomial coefficients $\binom{\tilde{\tau}_m}{k}$. Since $\nu^+(G, \sigma^I) = \nu^+(G, \sigma)$ and since, by Lemma 12, $|\text{FIX}(f)| \leq \phi(G, \sigma) = \phi(G, \sigma^I)$, this proves the theorem. \square

An equivalent statement is the one given in the introduction:

$$\phi(G, \sigma) \leq \sum_{k=\lfloor \frac{\tilde{\tau}_m - \nu^+}{2} \rfloor}^{\lfloor \frac{\tilde{\tau}_m + \nu^+}{2} \rfloor} \binom{\tilde{\tau}_m}{k}. \quad (17)$$

This clearly improves the bound 2^{τ^+} when $\tau^+ = \tilde{\tau}_m$ and when the gap between ν^+ and τ_m is large. Consider for instance the loop-less symmetric digraph K_n corresponding to the complete graph on $n \geq 2$ vertices, and let K_n^- be the signed digraph obtained from K_n by labeling negatively every arc. We have $\tau^+(K_n^-) = \tilde{\tau}_m(K_n^-) = n - 1 < \tau_m(K_n^-) = n$ and $\nu^+(K_n^-) = \lfloor \frac{n}{2} \rfloor$. Thus, by (17), $\phi(K_n^-)$ is at most the $\lfloor \frac{n}{2} \rfloor + 1$ largest binomial coefficient $\binom{n-1}{k}$. This is much better than the classical upper bound 2^{τ^+} which is, in that case, 2^{n-1} . However, for K_n^- , the upper bound (17) is still far from the exact value $\phi(K_n^-) = \binom{n}{\lfloor \frac{n}{2} \rfloor}$ established in [9] with a dedicated method. Actually, for K_n^- , the upper bound (17) is tight only for $n = 2, 3$ (while the bound 2^{τ^+} is tight only for $n = 2$).

Let us finally mention that the parameter $\tilde{\tau}_m$ is connected to the transversal number and frustration index in the following way. Let (G, σ) be a signed digraph and let I be such that (G, σ^I) has λ non-positive arcs. Let J be the set of vertices v such that G has an arc uv with $\sigma^I(uv) \neq 1$. If K is a feedback vertex set of G then $J \cup K$ is a monotone feedback vertex set of (G, σ^I) of size $|J \cup K| \leq |J| + |K| \leq \lambda + \tau$. Thus, for every signed digraph (G, σ) ,

$$\tau \leq \tilde{\tau}_m \leq \tau + \lambda.$$

5 Concluding remarks

Let us first remark that the parameters ν^* , ν and τ are invariant under the subdivision of arcs, and that the parameters ν^+ , τ^+ and τ_m and $\tilde{\tau}_m$ are invariant under the subdivision of arcs preserving signs (that is, when signed arcs are replaced by paths with the same signs). This is often relevant in practice. For instance, in biology, a biological pathways involving dozens of biological entities is often summarized by a single arc. Hence, in this kind of context, parameters invariant under subdivisions are particularly relevant, in contrast with the number of vertices, the circumference or the girth.

Let us now present a few possible future works. To make progresses on our understanding of $\phi_m(G)$, it could be interesting to determine the maximal size of a subset of $L \subseteq \{0, 1\}^\tau$ satisfying the four constraints of Theorem 2 (by Erdős' theorem, we know the maximal size of L subjects to the first two only). To initiate this study, it could be interesting to first focus on special k -patterns and to answer the following question: *Given positive integers k and n , what is the maximum size of a subset of $\{0, 1\}^n$ without special k -patterns.*

It could interesting to go further in the study of $\phi(G, \sigma)$, for instance by establishing lower bounds in the spirit of Theorem 4. We may also think about an improvement of (17) that generalizes (1) to the signed case.

Besides, we know that directed cycles have the Erdős-Pósa property: there exists a (small-est) function $h : \mathbb{N} \rightarrow \mathbb{N}$ such that $\tau \leq h(\nu)$ for every digraph [21]. This leads us to ask if non-negative cycles have also this property, that is: *Is there exists a function $h^+ : \mathbb{N} \rightarrow \mathbb{N}$ such that $\tau^+ \leq h^+(\nu^+)$ for every signed digraph?* It is easy to show that this is equivalent to ask if even directed cycles have the Erdős-Pósa property (this is true in the undirected case [29]).

Let $\phi_m(k)$ be the maximal number of $\phi_m(G)$ for a digraph G with $\nu(G) \leq k$. We know that $\phi_m(k)$ is finite for every k since, for every digraph G , we have $\phi_m(G) \leq 2^\tau \leq 2^{h(\nu)}$, so that $\phi_m(k) \leq 2^{h(k)}$. However, the established upper-bound on $h(k)$ is very large (power tower type) and the proof is quite involved. It could be thus interesting to try to prove the finiteness of $\phi_m(k)$ directly, without use the fact that directed cycles have the Erdős-Pósa property. We could hope to find, in this way, the right order of magnitude of $\phi_m(k)$. Let us mention that, according to (2), $\phi_m(1) = 2$, and according to the proposition below, $\phi_m(2) = 4$. In contrast, the unique exact value of h is $h(1) = 3$ and is very hard to obtain [20]. This shows that bounding ϕ_m by ν could be much more simple than bounding τ by ν .

Proposition 4. *For every digraph G ,*

$$\nu \leq 2 \Rightarrow \phi_m(G) \leq 4.$$

Proof. Let f be a monotone network with interaction graph G . We first prove the following: *If f has three pairwise incomparable fixed points, then G has three vertex-disjoint cycles.* Let x^1, x^2, x^3 be three pairwise incomparable fixed points of f . Let

$$V_1 = \{v : x_v^1 > x_v^2\}, \quad V_2 = \{v : x_v^2 > x_v^3\}, \quad V_3 = \{v : x_v^3 > x_v^1\}.$$

It is easy to see that V_1, V_2 and V_3 are pairwise disjoint and that, for $i = 1, 2, 3$, the minimal in-degree of $G[V_i]$ is at least one. Thus G has three vertex-disjoint cycles. Therefore, if $\nu \leq 2$, then $\text{FIX}(f)$ has no antichain of size 3 and no chain of size 4 (cf. Lemma 3). Since $\text{FIX}(f)$ is a lattice, we deduce that f has at most four fixed points (and this bound is sharp, as showed by the identity on $\{0, 1\}^2$). \square

References

- [1] R. Ahlswede, Ning Cai, S.-Y.R. Li, and R.W. Yeung. Network information flow. *Information Theory, IEEE Transactions on*, 46(4):1204–1216, Jul 2000.
- [2] R. Albert. Boolean modeling of genetic regulatory networks. In Eli Ben-Naim, Hans Frauenfelder, and Zoltan Toroczkai, editors, *Complex Networks*, volume 650 of *Lecture Notes in Physics*, pages 459–481. Springer Berlin Heidelberg, 2004.
- [3] J. Aracena. Maximum number of fixed points in regulatory Boolean networks. *Bulletin of Mathematical Biology*, 70(5):1398–1409, 2008.
- [4] J. Aracena, A. Richard, and L. Salinas. Maximum number of fixed points in AND-OR-NOT networks. *Journal of Computer and System Sciences*, 80(7):1175 – 1190, 2014.
- [5] S. Bornholdt. Boolean network models of cellular regulation: prospects and limitations. *Journal of The Royal Society Interface*, 5(Suppl 1):S85–S94, 2008.
- [6] Paul Erdős. On a lemma of littlewood and offord. *Bulletin of the American Mathematical Society*, 51(12):898–902, 1945.

- [7] Péter L Erdos, Zoltán Füredi, and Gyula OH Katona. Two-part and k-sperner families: new proofs using permutations. *SIAM Journal on Discrete Mathematics*, 19(2):489–500, 2005.
- [8] M. Gadouleau, A. Richard, and E. Fanchon. Reduction and Fixed Points of Boolean Networks and Linear Network Coding Solvability. *ArXiv e-prints*, December 2014.
- [9] M. Gadouleau, A. Richard, and S. Riis. Fixed points of Boolean networks, guessing graphs, and coding theory. *To appear in SIAM Journal on Discrete Mathematics*, 29(4):2312–2335, 2015.
- [10] M. Gadouleau and S. Riis. Graph-theoretical constructions for graph entropy and network coding based communications. *IEEE Transactions on Information Theory*, 57(10):6703–6717, 2011.
- [11] Bertrand Guenin and Robin Thomas. Packing directed circuits exactly. *Combinatorica*, 31(4):397–421, 2011.
- [12] Frank Harary. On the measurement of structural balance. *Behavioral Science*, 4(4):316–323, 1959.
- [13] Teresa W Haynes, Stephen Hedetniemi, and Peter Slater. *Fundamentals of domination in graphs*. CRC Press, 1998.
- [14] J. Hopfield. Neural networks and physical systems with emergent collective computational abilities. *Proc. Nat. Acad. Sc. U.S.A.*, 79:2554 – 2558, 1982.
- [15] S. A. Kauffman. Metabolic stability and epigenesis in randomly connected nets. *Journal of Theoretical Biology*, 22:437–467, 1969.
- [16] S. A. Kauffman. *Origins of Order Self-Organization and Selection in Evolution*. Oxford University Press, 1993.
- [17] Nicolas Le Novère. Quantitative and logic modelling of molecular and gene networks. *Nature Reviews Genetics*, 16:146–158, 2015.
- [18] Changwoo Lee. Domination in digraphs. *J. Korean Math. Soc*, 35(4):843–853, 1998.
- [19] W. S. Mac Culloch and W. S. Pitts. A logical calculus of the ideas immanent in nervous activity. *Bull. Math Bio. Phys.*, 5:113 – 115, 1943.
- [20] William McCuaig. Intercyclic digraphs. *Contemporary Mathematics*, 147:203–245, 1993.
- [21] Bruce Reed, Neil Robertson, Paul Seymour, and Robin Thomas. Packing directed circuits. *Combinatorica*, 16(4):535–554, 1996.
- [22] E. Remy, P. Ruet, and D. Thiéffry. Graphic requirements for multistability and attractive cycles in a Boolean dynamical framework. *Advances in Applied Mathematics*, 41(3):335 – 350, 2008.
- [23] S. Riis. Information flows, graphs and their guessing numbers. *The Electronic Journal of Combinatorics*, 14:1–17, 2007.
- [24] F. Robert. *Discrete iterations: a metric study*, volume 6 of *Series in Computational Mathematics*. Springer, 1986.

- [25] Paul D. Seymour. Packing directed circuits fractionally. *Combinatorica*, 15(2):281–288, 1995.
- [26] R. Thomas. Boolean formalization of genetic control circuits. *Journal of Theoretical Biology*, 42(3):563 – 585, 1973.
- [27] R. Thomas and R. d’Ari. *Biological Feedback*. CRC Press, 1990.
- [28] R. Thomas and M. Kaufman. Multistationarity, the basis of cell differentiation and memory. II. Logical analysis of regulatory networks in terms of feedback circuits. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 11(1):180–195, 2001.
- [29] Carsten Thomassen. On the presence of disjoint subgraphs of specified type. *Journal of Graph Theory*, 12:101–111, 1988.
- [30] Thomas Zaslavsky. Signed graphs. *Discrete Applied Mathematics*, 4(1):47–74, 1982.
- [31] Thomas Zaslavsky. A mathematical bibliography of signed and gain graphs and allied areas. *The Electronic Journal of Combinatorics*, 1000:DS8–Sep, 2012.

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