

Isomorphic Boolean networks and dense interaction graphs

Aymeric Picard, Adrien Richard

▶ To cite this version:

Aymeric Picard, Adrien Richard. Isomorphic Boolean networks and dense interaction graphs. Automata 2021, Jul 2021, Marseille, France. hal-03235769

HAL Id: hal-03235769

https://hal.science/hal-03235769

Submitted on 26 May 2021

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Isomorphic Boolean networks and dense interaction graphs

Aymeric Picard Marchetto* and Adrien Richard*

May 26, 2021

Abstract

A Boolean network (BN) with n components is a discrete dynamical system described by the successive iterations of a function $f:\{0,1\}^n \to \{0,1\}^n$. In most applications, the main parameter is the interaction graph of f: the digraph with vertex set $\{1,\ldots,n\}$ that contains an arc from j to i if f_i depends on input j. What can be said on the set $\mathcal{G}(f)$ of the interaction graphs of the BNs h isomorphic to f, that is, such that $h \circ \pi = \pi \circ f$ for some permutation π of $\{0,1\}^n$? It seems that this simple question has never been studied. Here, we report some basic facts. First, if $n \geq 5$ and f is neither the identity or constant, then $\mathcal{G}(f)$ is of size at least two and contains the complete digraph on n vertices, with n^2 arcs. Second, for any $n \geq 1$, there are n-component BNs f such that every digraph in $\mathcal{G}(f)$ has at least $n^2/9$ arcs.

1 Introduction

A Boolean network (network for short) with n components is a finite dynamical system defined by the successive iterations of a function

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

Boolean networks have many applications; in particular, they are omnipresent in the modeling of neural and gene networks (see [4] for a review).

The "network" terminology comes from the fact that the interaction graph G(f) of f is often considered as the main parameter of f: the vertex set is $[n] = \{1, ..., n\}$ and there is an arc from f to f if f depends on input f, that is, if there are f is an arc from f to f if f is a such that f if there are f in the context of gene networks, the interaction graph is often well approximated while the actual dynamics is not. One is thus faced with the following question: what can be said on the dynamics

^{*}Laboratoire I3S, UMR CNRS 7271 & Université Côte d'Azur, France. This work is supported by the Young Researcher project ANR- 18-CE40-0002-01 "FANs" and project STIC AmSud CoDANet 19-STIC-03 (Campus France 43478PD).

described by f from G(f) only. There are many results in this direction (see [1] for a review). In most cases, the studied dynamical properties are invariant by isomorphism: number of fixed or periodic points, number and size of limit cycles, transient length and so on. However, the interaction graph is not invariant by isomorphism: even if f and h are isomorphic, their interaction graphs can be very different (by Theorem 1 below, G(f) can have n^2 arcs while G(h) has a single arc). Surprisingly, this variation seems to have never been studied, and we report here some basic facts.

Given a network f, let $\mathcal{G}(f)$ be the set of interaction graphs G(h) such that h is a network isomorphic to f, that is, such that $h \circ \pi = \pi \circ f$ for some permutation π of $\{0,1\}^n$. Hence, we propose to study $\mathcal{G}(f)$. For instance, if f is constant, we write this f = cst, then $\mathcal{G}(f)$ contains a single digraph, the digraph on [n] without arcs, and if f is the identity, we write this f = id, then $\mathcal{G}(f)$ also contains a single digraph, the digraph on [n] with n loops (cycles of length one) and no other arcs.

Our first result shows that, excepted few exceptions (including the two above examples), $\mathcal{G}(f)$ always contains the complete digraph on [n], with n^2 arcs, denoted K_n .

Theorem 1. $K_n \in \mathcal{G}(f)$ for all networks $f \neq \text{cst}$, id with $n \geq 5$ components.

Our second result shows that, for $n \geq 5$, there are no networks f such that $\mathcal{G}(f)$ only contains the complete digraph.

Theorem 2. $\mathcal{G}(f) \neq \{K_n\}$ for all networks f with $n \geq 5$ components.

From these theorems we deduce the following property, which might seem innocente but that doesn't seem to have a one-line proof: If f is a network with $n \ge 5$ components, then $|\mathcal{G}(f)| = 1$ if and only if f = id or f = cst.

Even if, for $n \geq 5$, $\mathcal{G}(f)$ cannot only contain the complete digraph, using a well-known isoperimetric inequality in hypercubes, we show that, at least, $\mathcal{G}(f)$ can only contain digraphs with many arcs.

Theorem 3. For every $n \ge 1$, there is a network f with n components such that every digraph in $\mathcal{G}(f)$ has at least $n^2/9$ arcs.

Concerning short term perspectives, we checked by computer that the first theorem holds for n=3 (for n=2 it fails; see the appendix) and that the second holds for n=2,3. For n=4 this is much time-consuming and we didn't do it, hoping to find instead dedicated arguments, since those given for $n\geq 5$ do not work. A more involved perspective, related to the third theorem, is to prove that, for any $\epsilon>0$ and n large enough, any digraph in $\mathcal{G}(f)$ has at least $(1-\epsilon)n^2$ arcs for some f. We also want to study networks f such that $\mathcal{G}(f)$ is very large and ask: do we have, for any $\epsilon>0$ and n large enough, $|\mathcal{G}(f)|/2^{n^2}>1-\epsilon$ for some f?

The three theorems above are proved the in following three sections. Before going on, we give some basic definitions. An element x of $\{0,1\}^n$ is a

configuration, and elements in [n] are components. We set $\mathbf{1}(x) = \{i \in [n] \mid x_i = 1\}$ and $\mathbf{0}(x) = [n] \setminus \mathbf{1}(x)$. The weight of x is $w(x) = |\mathbf{1}(x)|$. We denote by e_i the configuration such that $\mathbf{1}(e_i) = \{i\}$. For $x, y \in \{0, 1\}^n$, the sum x + y is applied component-wise modulo two. Hence x and $x + e_i$ only differ in component i. We denote by $\mathbf{1}$ (resp. $\mathbf{0}$) the configuration of weight n (resp. 0). Thus x and $x + \mathbf{1}$ differ in every component. Given $A \subseteq \{0, 1\}^n$, we set $A + x = \{a + x \mid a \in A\}$. Let f be a n-component network. A fixed point is a configuration x such that f(x) = x. Let $\Gamma(f)$ be the digraph with vertex set $\{0, 1\}^n$ and an arc from x to f(x) for every $x \in \{0, 1\}^n$. A limit cycle of f is a cycle of $\Gamma(f)$. Hence fixed points correspond to limit cycles of length one. An independent set of f is an independent set of f, equivalently, it is a set f is a set f is an independent set of f.

2 Proof of Theorem 1

We proceed by showing that, for $n \geq 5$ and $f \neq \text{cst}$, id, we have $K_n \in \mathcal{G}(f)$ if at least one of the following three conditions holds: f has at least 2n fixed points; or f has at least n limit cycles of length ≥ 3 ; or f has an independent set of size $\geq 2n$. We then prove that, because $n \geq 5$, at least one of the three conditions holds, and Theorem 1 follows.

Lemma 1. Let f be a network with n components, which is not the identity. If f has at least 2n fixed points then $K_n \in \mathcal{G}(f)$.

Proof. Since $f \neq \text{id}$ we have $f(c) \neq c$ for some c, and since f has at least 2n fixed points, it has 2n-1 fixed points distinct from f(c), say $a^0, a^1, \ldots, a^n, b^3, \ldots, b^n$. Let π be any permutation of $\{0, 1\}^n$ such that $\pi(a^0) = \mathbf{0}$, $\pi(a^i) = e_i$ for $1 \leq i \leq n$, $\pi(b^i) = e_1 + e_2 + e_i$ for $3 \leq i \leq n$, $\pi(c) = e_1 + e_2$ and $\pi(f(c)) = e_1 + e_2 + \mathbf{1}$. Let $h = \pi \circ f \circ \pi^{-1}$. We will prove that $G(h) = K_n$. For $i \in [n]$, we have $h(\mathbf{0}) = \pi(f(a^0)) = \pi(a^0) = \mathbf{0}$ and $h(e_i) = \pi(f(a^i)) = \pi(a^i) = e_i$, hence $h(\mathbf{0})$ and $h(e_i)$ differ in component i, and we deduce that G(h) has an arc from i to itself. It remains to prove that G(h) has an arc from i to j for distinct $i, j \in [n]$. We have $h(e_1 + e_2) = \pi(f(c)) = e_1 + e_2 + \mathbf{1}$. Hence $h(e_2) = e_2$ and $h(e_1 + e_2)$ differ in every component $j \neq 1$, and thus G(h) has an arc from 1 to every $j \neq 1$. We prove similarly that G(h) has an arc from 2 to every $j \neq 2$. For $3 \leq i \leq n$, we have $h(e_1 + e_2 + e_i) = \pi(f(b^i)) = \pi(b^i) = e_1 + e_2 + e_i$, so $h(e_1 + e_2 + e_i)$ and $h(e_1 + e_2)$ differ in every component $j \neq i$, and we deduce that G(h) has an arc from i to every $j \neq i$.

Lemma 2. Let f be a network with n components. If f has at least n limit cycles of length ≥ 3 , then $K_n \in \mathcal{G}(f)$.

Proof. Suppose that f has n limit cycles of length ≥ 3 ; this implies $n \geq 4$. Let a^1, \ldots, a^n be configurations inside distinct limit cycles of f of length

 ≥ 3 . For $i \in [n]$ let $b^i = f(a^i)$ and $c^i = f(b^i)$. Then $a^1, \ldots, a^n, b^1, \ldots, b^n, c^1, \ldots, c^n$ are all distinct. For $i \in [n]$, let $x^i = e_{i-1} + e_i, \ y^i = e_{i-1}$ and $z^i = e_{i-1} + 1$, where e_0 means e_n . Since $n \geq 4$, the configurations $x^1, \ldots, x^n, y^1, \ldots, y^n, z^1, \ldots, z^n$ are all distinct. Hence there is a permutation π of $\{0,1\}^n$ such that, for $i \in [n]$, $\pi(a^i) = x^i, \pi(b^i) = y^i$ and $\pi(c^i) = z^i$. Let $h = \pi \circ f \circ \pi^{-1}$. For $i \in [n]$ we have $h(e_{i-1} + e_i) = h(x^i) = \pi(f(a^i)) = \pi(b^i) = y^i = e_{i-1}$ and $h(e_{i-1}) = h(y^i) = \pi(f(b^i)) = \pi(c^i) = z^i = e_{i-1} + 1$. Hence $h(e_{i-1} + e_i)$ and $h(e_{i-1})$ differ in every component, and since $e_{i-1} + e_i$ and e_{i-1} only differ in component i, we deduce that G(h) has an arc from i to every $j \in [n]$. Thus $G(h) = K_n$.

Lemma 3. Let f be a non-constant network with $n \geq 5$ components. If f has an independent set of size $\geq 2n$, then $K_n \in \mathcal{G}(f)$.

Proof. Let A be an independent set of f. We first prove:

(1) If
$$|A| \ge n + k$$
 and $|f(A)| = 2k$ for some $1 \le k \le n$, then $K_n \in \mathcal{G}(f)$.

Suppose these condition holds. One easily check that there is an independent set A with |A| = n + k and |f(A)| = 2k for some $1 \le k \le n$. Let us write $f(A) = \{a^1, \ldots, a^{2k}\}$, and let $A_p = f^{-1}(a^p) \cap A$ for $p \in [2k]$. Let X_1, \ldots, X_{2k} be disjoint subsets of $\{0, 1\}^n$ of size $|A_1|, \ldots, |A_{2k}|$ such that, for all $i \in [n]$, there is $p \in [k]$ and $x \in X_{2p-1}$ with $x + e_i \in X_{2p}$; that these sets exist is the "technical" part of the proof, given by Lemma 8 in appendix.

Let $X = X_1 \cup \cdots \cup X_{2k}$, let Y be the set of $y \in \{0,1\}^n$ with $y_1 = 0$, and let Y' be the set of $y \in Y$ such that $y, y + 1 \notin X$. Since $n \geq 5$ and $n \geq k$:

$$|Y'| > |Y| - |X| = 2^{n-1} - (n+k) > 2^{n-1} - 2n > n > k.$$

Thus there are k distinct configurations in $y^1, \ldots, y^k \in Y'$ and by construction, $Y'' = \{y^1, \ldots, y^k\}$ and $Y'' + \mathbf{1}$ are disjoint and disjoint from X.

Hence there is a permutation π of $\{0,1\}^n$ such that, for all $p \in [k]$, $\pi(a^{2p-1}) = y^p$, $\pi(a^{2p}) = y^p + 1$, $\pi(A_{2p-1}) = X_{2p-1}$ and $\pi(A_{2p}) = X_{2p}$. Let $h = \pi \circ f \circ \pi^{-1}$. By construction, for every $i \in [n]$ there is $p \in [k]$ and $x \in X_{2p-1}$ with $x+e_i \in X_{2p}$. Since $\pi^{-1}(x) \in A_{2p-1}$ and $\pi^{-1}(x+e_i) \in A_{2p}$, we have $h(x) \in \pi(f(A_{2p-1})) = \{\pi(a^{2p-1})\} = \{y^p\}$ and $h(x+e_i) \in \pi(f(A_{2p})) = \{\pi(a^{2p})\} = \{y^p + 1\}$. Thus h(x) and $h(x+e_i)$ differ in every component, and we deduce that $G(h) = K_n$. This proves (1).

We next prove another condition on A to obtain the complete digraph.

(2) If
$$|A| > n$$
 and $|f(A)| = 1$, then $K_n \in \mathcal{G}(f)$.

Let $a \in \{0,1\}^n$ such that $f(A) = \{a\}$. Since $f \neq \text{cst}$, there is $b \in \{0,1\}^n$ with $f(b) \neq a$, and thus $b \notin A$. We consider three cases.

Suppose first that $f(a) \neq a$. Since |A| > n, there are *n* configurations a^1, \ldots, a^n in *A* distinct from f(a). Then $a^1, \ldots, a^n, a, f(a)$ are all distinct, so

there is a permutation π with $\pi(a) = \mathbf{0}$, $\pi(f(a)) = \mathbf{1}$ and $\pi(a^i) = e_i$ for $1 \le i \le n$. Let $h = \pi \circ f \circ \pi^{-1}$. For $i \in [n]$, we have $h(e_i) = \pi(f(a^i)) = \pi(a) = \mathbf{0}$ and $h(\mathbf{0}) = \pi(f(a)) = \mathbf{1}$, so $h(e_i)$ and $h(\mathbf{0})$ differ in every component, and thus $G(h) = K_n$.

Suppose now that f(a) = a and f(b) = b. Let $a^1, \ldots, a^n \in A$, all distinct. Then a^1, \ldots, a^n, a, b are all distinct since $b = f(b) \neq a$. So there is a permutation π with $\pi(a) = \mathbf{1}$, $\pi(b) = \mathbf{0}$ and $\pi(a^i) = e_i$ for $i \in [n]$. Let $h = \pi \circ f \circ \pi^{-1}$. For all $i \in [n]$, we have $h(e_i) = \pi(f(a^i)) = \pi(a) = \mathbf{1}$ and $h(\mathbf{0}) = \pi(f(b)) = \pi(b) = \mathbf{0}$, so $h(e_i)$ and $h(\mathbf{0})$ differ in every component, and thus $G(h) = K_n$.

Suppose finally that f(a) = a and $f(b) \neq b$. Since |A| > n, there is $A' \subseteq A \setminus \{f(b)\}$ of size n. Then $A' \cup \{b\}$ is an independent set of size n+1 and $|f(A' \cup \{b\})| = |\{a, f(b)\}| = 2$ so $K_n \in \mathcal{G}(f)$ by (1). This proves (2).

We can now conclude the proof. Suppose that $|A| \geq 2n$. Then we can choose A so that |A| = 2n. Suppose, for a contradiction, that $K_n \notin \mathcal{G}(f)$. If |f(A)| is even then $K_n \in \mathcal{G}(f)$ by (1) and if |f(A)| = 1 then $K_n \in \mathcal{G}(f)$ by (2). Thus |f(A)| = 2k + 1 for some $1 \leq k < n$. Let us write $f(A) = \{a^1, \ldots, a^{2k+1}\}$, and let $A_p = f^{-1}(a^p) \cap A$ for $1 \leq p \leq 2k + 1$. Suppose, without loss, that $|A_1| \leq |A_2| \leq \cdots \leq |A_{2k+1}|$. Then $A' = A \setminus A_1$ is an independent set with |f(A')| = 2k. Setting m = n + k - 1, if |A'| > m, then $K_n \in \mathcal{G}(f)$ by (2). So $2k|A_2| \leq |A'| \leq m$, thus $|A_1| \leq |A_2| \leq m/2k$. We deduce that $2n = |A| = |A_1| + |A'| \leq m/2k + m$. However, one easily checks that 2n > m/2k + m when $1 \leq k < n$, a contradiction. Thus $K_n \in \mathcal{G}(f)$

We are ready to prove Theorem 1. Let $f \neq \text{cst}$, id with $n \geq 5$ components. Suppose, for a contradiction, that $K_n \notin \mathcal{G}(f)$. Let F be the set of fixed points of f, and let L be a smallest subset of $\{0,1\}^n$ intersecting every limit cycle of f of length ≥ 3 . Let Γ' be obtained from $\Gamma(f)$ by deleting the vertices in $F \cup L$; then Γ' has only cycles of length two, thus it is bipartite. Since $K_n \notin \mathcal{G}(f)$, by Lemmas 1 and 2, we have |F| < 2n and |L| < n, thus Γ' has at least $N = 2^n - 3n + 2$ vertices. Since Γ' is bipartite, it has an independent set A of size $\geq N/2$. Then A is an independent set of f and since $K_n \notin \mathcal{G}(f)$, we deduce from Lemma 3 that |A| < 2n. Thus 2n > N/2, that is, $7n > 2^n + 3$, which is false since $n \geq 5$. Thus $K_n \in \mathcal{G}(f)$.

3 Proof of Theorem 2

We first give a necessary and sufficient condition for the presence of a digraph in $\mathcal{G}(f)$ that misses some arc with distinct ends. It has been obtained with Kévin Perrot, whom we thank, and its proof is in appendix. Given an n-component network f, and $1 \leq k \leq 2^{n-1}$, a k-nice set of f is a set $A \subseteq \{0,1\}^n$ of size 2k with $|f^{-1}(A)|$ and $|f^{-1}(A) \cap A|$ even.

Lemma 4. Let f be an n-component network and distinct $i, j \in [n]$. Some digraph in $\mathcal{G}(f)$ has no arc from j to i if and only if f has a (2^{n-2}) -nice set.

Hence, to prove Theorem 2, it is sufficient to prove that, for $n \geq 5$, f has always a (2^{n-2}) -nice set. To use induction, it is more convenient to prove something stronger: if $n \geq 4$ and $8 \leq k \leq 2^{n-1}$ then f has always a k-nice set. In particular, if $n \geq 5$ then $2^{n-2} \geq 8$ thus f has a (2^{n-2}) -nice set and we are done. So it remains to prove:

Lemma 5. Let f be a network with $n \ge 4$ components and $8 \le k \le 2^{n-1}$. Then f has a k-nice set.

Proof. We proceed by induction on k, decreasing from 2^{n-1} to 8. For the base case, observe that $\{0,1\}^n$ is a (2^{n-1}) -nice set of f. Suppose that $8 < k \le 2^{n-1}$, and suppose that f has a k-nice set A. We will prove that f has a (k-1)-nice set included in A, thus completing the induction step. For that, we will define an equivalence relation on A, with at most 8 equivalence classes, and show that, since $A \ge 18$, there always are two equivalent elements $x, y \in A$ such that $A \setminus \{x, y\}$ is a (k-1)-nice set of f. This relation is defined through 3 binary properties on the elements of A, defined below.

Let $\alpha, \beta, \gamma : A \to \{0, 1\}$ be defined by: for all $x \in A$,

- 1. $\alpha(x) = 1$ if and only if $f(x) \in A$,
- 2. $\beta(x) = 1$ if and only if $|f^{-1}(x)|$ is even,
- 3. $\gamma(x) = 1$ if and only if $|(f^{-1}(x) \cap A) \setminus \{x\}|$ is even.

We say that $x, y \in A$ are equivalent if $\alpha(x) = \alpha(y)$ and $\beta(x) = \beta(y)$ and $\gamma(x) = \gamma(y)$. We say that $x, y \in A$ are independent if $f(x) \neq y$ and $f(y) \neq x$. It is straightforward (and annoying) to check that if $x, y \in A$ are equivalent and independent, then $A \setminus \{x, y\}$ is a (k-1)-nice of f.

Suppose now that f has no (k-1)-nice set. By the above property, there is no equivalence class containing two independent elements. Let $A_0 = \alpha^{-1}(0)$ and $A_1 = \alpha^{-1}(1)$. Each of A_0, A_1 contains at most 4 equivalence classes. If $x, y \in A_0$, then $f(x), f(y) \notin A$, and thus x and y are independent. We deduce that each of the classes contained in A_0 is of size < 2, and thus $|A_0| \le 4$. Also, one easily checks that any class of size ≥ 4 contains two independent elements. Hence each of the classes contained in A_1 is of size < 4, and thus $|A_1| \le 12$. But then $|A| = |A_1| + |A_2| \le 16$, a contradiction. Thus f has a (k-1)-nice set.

4 Proof of Theorem 3

If $1 \le n \le 9$ and f is the identity on $\{0,1\}^n$, then $\mathcal{G}(f)$ contains a unique digraph, which has $n = n^2/n \ge n^2/9$ vertices. This proves the theorem for $n \le 9$. We treat the other cases with an explicit construction.

Given $A \subseteq \{0,1\}^n$ with $\mathbf{0} \in A$, we denote by f^A the *n*-component network such that $f^A(A) = \{\mathbf{0}\}$ and $f^A(b) = b$ for all $b \notin A$. We will prove, in the next lemma, that if the size of A is carefully chosen, then, independently on the structure of A, $G(f^A)$ has at least $n^2/9$ arcs. It is then easy to prove that this lower bound holds for every digraph in $\mathcal{G}(f^A)$.

Lemma 6. Let $n \geq 9$ and $A \subseteq \{0,1\}^n$ of size $\lceil 2^{n/4} \rceil$ with $\mathbf{0} \in A$. Then $G(f^A)$ has at least $n^2/9$ arcs.

The key tool is the following lemma, which can be easily deduced from the well-known Harper's isoperimetric inequality in the hypercube (see the appendix). Let Q_n be the hypercube graph, with vertex set $\{0,1\}^n$ and an edge between x and y if and only if x and y differ in exactly one component.

Lemma 7. Let $A \subseteq \{0,1\}^n$ be non-empty, and let d be the average degree of the subgraph of Q_n induced by A. Then $|A| \ge 2^d$.

Proof of Lemma 6. Let $f = f^A$ and let m be the number of arcs in G(f). Suppose, for a contradiction that $m < n^2/9$. Let I be the set of $i \in [n]$ with $a_i = 1$ for some $a \in A$. Note that $|I| \ge n/4$. Indeed, let B be the set of $b \in \{0,1\}^n$ such that $b_i = 0$ for all $i \notin I$. Then $A \subseteq B$, and $|B| = 2^{|I|}$, thus $|I| = \log_2 |B| \ge \log_2 |A| \ge n/4$. From that observation, we can say something stronger:

(1)
$$|I| > n/2$$
.

Let $i \in I$ and $j \notin I$. Let $a \in A$ such that $a_i = 1$. Since $j \notin I$, $a + e_j \notin A$, thus $f(a) = \mathbf{0}$ and $f(a + e_j) = a + e_i$, and $f_i(a + e_j) = a_i = 1$ since $j \neq i$. Hence G(f) has an arc from j to i. We deduce that $|I| \cdot (n - |I|) \le m < n^2/9$, so $n/4 \cdot (n - |I|) < n^2/9$. Thus |I| > 5n/9 > n/2. This proves (1).

We deduce that some $a \in A$ has a large weight.

(2) There is $a \in A$ with w(a) > 3n/4.

Suppose that $w(a) \leq 3n/4$ for all $a \in A$. Let $i \in I$. Let $a \in A$ with $a_i = 1$, and w(a) maximal for that property. Then, for all $j \in \mathbf{0}(a)$, we have $a + e_j \notin A$. Hence $f(a) = \mathbf{0}$ and $f(a + e_j) = a + e_j$ so $f_i(a + e_j) = a_i = 1$ since $i \neq j$. Thus G(f) has an arc from j to i. We deduce that the in-degree of i in G(f) is at least $|\mathbf{0}(a)| = n - w(a) \geq n/4$. Hence $m \geq |I| \cdot n/4$ and since |I| > n/2 by (1) we obtain $m > n^2/8 > n^2/9$, a contradiction. This proves (2).

Let A' be the set of $a \in A$ with $w(a) \ge n/3 - 1$, which is not empty by (2). For $a \in A$, let J(a) be the set of $j \in [n]$ such that $a + e_j \in A$, and let J'(a) be the set of $j \in [n]$ such that $a + e_j \in A'$. Let H be the subgraphs of Q_n induced by A'. If $a \in A'$, then d(a) = |J'(a)| is the degree of a in H. We will prove in (3) and (4) below that each vertex in H has large degree.

(3) If $a \in A'$ and $w(a) \ge n/3$ then d(a) > n/3.

Indeed, since $w(a) \ge n/3$, for $j \in J(a)$ we have $w(a + e_j) \ge n/3 - 1$ thus $j \in J'(a)$. Hence J(a) = J'(a) so d(a) = |J(a)|. For all $i \notin J(a)$ we have $f(a) = \mathbf{0}$ and $f(a + e_i) = a + e_i$, thus G(f) has an arc from i to each component in $\mathbf{1}(a + e_i)$. Thus the out-degree of i in G(f) has at least $w(a + e_i) \ge n/3 - 1$. We deduce that $(n - |J(a)|) \cdot (n/3 - 1) \le m < n^2/9$, so d(a) = |J(a)| > 2n/3 - 3 and since $n \ge 9$ we obtain d(a) > n/3. This proves (3).

(4) If $a \in A'$ and w(a) < n/3 then d(a) > n/3.

Let $K = \mathbf{0}(a) \setminus J'(a)$ and $i \in K$. We have $w(a + e_i) = w(a) + 1 \ge n/3$, thus if $a + e_i \in A$ then $a + e_i \in A'$; but then $i \in J'(a)$, a contradiction. Thus $a + e_i \notin A$, so $f(a) = \mathbf{0}$ and $f(a + e_i) = a + e_i$. We deduce that the out-degree of i in G(f) is at least $w(a + e_i) \ge n/3$. Thus $|K| \cdot n/3 \le m < n^2/9$ so |K| < n/3. Since w(a) < n/3 we have $|\mathbf{0}(a)| > 2n/3$. So $|K| \ge 2n/3 - |J'(a)|$ and thus d(a) = |J'(a)| > n/3. This proves (4).

We are now in position to finish the proof. Let d be the average degree of H. By (3) and (4), we have d > n/3. Using Lemma 7 we obtain $2^{n/3} < 2^d \le |A'| \le |A| = \lceil 2^{n/4} \rceil$, which is false because $n \ge 9$.

We are now in position to conclude. Let $n \geq 9$ and $A \subseteq \{0,1\}^n$ of size $\lceil 2^{n/4} \rceil$ with $\mathbf{0} \in A$, and let $f = f^A$. Let π be any permutation of $\{0,1\}^n$ and $h = \pi \circ f \circ \pi^{-1}$. We will prove that G(h) has at least $n^2/9$ arcs. Let h' be the n-component network defined by $h'(x) = h(x + \pi(\mathbf{0})) + \pi(\mathbf{0})$ for all $x \in \{0,1\}^n$. We have G(h) = G(h'). Let $A' = \pi(A) + \pi(\mathbf{0})$. We have $\mathbf{0} \in A'$ and one easily check that $h' = f^{A'}$. Since $|A'| = |A| = \lceil 2^{n/4} \rceil$, by Lemma 6, G(h') = G(h) has at least $n^2/9$ arcs.

References

- [1] Maximilien Gadouleau. On the influence of the interaction graph on a finite dynamical system. *Natural Computing*, 19(1):15–28, 2020.
- [2] Lawrence Hueston Harper. Optimal assignments of numbers to vertices. Journal of the Society for Industrial and Applied Mathematics, 12(1):131–135, 1964.
- [3] Jeff Kahn and Jinyoung Park. An isoperimetric inequality for the hamming cube and some consequences. *Proceedings of the American Mathematical Society*, 148(10):4213–4224, 2020.
- [4] Nicolas Le Novère. Quantitative and logic modelling of molecular and gene networks. *Nature Reviews Genetics*, 16:146–158, 2015.

A Examples

Consider the 6 following networks with two components, denoted from f^1 to f^6 (each is given under three forms: a table, a graph, and formulas).

One can check that, given a network $f \neq \text{cst}$, id with 2 components: $K_2 \notin \mathcal{G}(f)$ if and only if f is isomorphic to one of the networks given above. Thus

these 6 networks are the counter examples of Theorem 1 for n=2. For instance, there are 6 networks isomorphic to f^1 , denoted from h^1 to h^6 (with $h^1 = f^1$, given below with their interactions graphs. We deduce that $\mathcal{G}(f^1)$ contains three digraphs, each distinct from K_2 .

A corollary of Theorems 1 and 2, stated in the introduction, is that,

for any network f with $n \geq 5$ components, we have $|\mathcal{G}(f)| = 1$ if and only if f = id or f = cst. This is also true for n = 3 (checked by computer) and open for n = 4. But for n = 2, f^2 is a counter example, the only one with two components. Indeed, there are 3 networks isomorphic to f^2 , denoted from g^1 to g^3 (with $g^1 = f^2$), given below, and they have the same interaction graph, with a loop on each vertex, as for the identity.

\mathbf{B} Lemma for the proof of Theorem 1

01

10 11 10 01

00

Lemma 8. Let $1 \le k \le n$ and let s_1, \ldots, s_{2k} be positive integers with sum equal to n+k. If $n \geq 5$, then there are disjoint subsets $X_1, \ldots, X_{2k} \subseteq \{0,1\}^n$ of size s_1, \ldots, s_{2k} such that, for every $i \in [n]$, there is $p \in [k]$ and $x \in X_{2p-1}$ with $x + e_i \in X_{2p}$.

Proof. Let I_1, \ldots, I_{2k} be a partition of [n] (with some members possibly empty) such that, for $1 \le \ell \le 2k$, the size of I_{ℓ} is $s_{\ell} - 1$ if ℓ is odd, and s_{ℓ} otherwise; it exists since the sum of the s_{ℓ} is n+k. For $1 \leq p \leq k$, select a configuration $x^{2p-1} \in \{0,1\}^n$, a component $j_{2p} \in I_{2p}$, and let

$$\begin{array}{rcl} X_{2p-1} & = & \{x^{2p-1}\} \cup \{x^{2p-1} + e_{j_{2p}} + e_i \mid i \in I_{2p-1}\}, \\ X_{2p} & = & \{x^{2p-1} + e_i \mid i \in I_{2p}\}. \end{array}$$

Clearly, $|X_{2p-1}| = |I_{2p-1}| + 1 = s_{2p-1}$ and $|X_{2p}| = |I_{2p}| = s_{2p}$. Let $i \in [n]$. Then $i \in I_{\ell}$ for some $1 \le \ell \le 2k$. If $\ell = 2p-1$ then, setting $x = x^{2p-1} + 2k$ $e_{j_{2p}} + e_i$, we have $x \in X_{2p-1}$ and $x + e_i = x^{2p-1} + e_{j_{2p}} \in X_{2p}$. If $\ell = 2p$ then, setting $x = x^{2p-1}$, we have $x \in X_{2p-1}$ and $x + e_i \in X_{2p}$. Thus we only have to prove that we can choose the configurations x^{2p-1} so that the sets X_1, \ldots, X_{2k} are pairwise disjoint. This is obvious if k=1 (and it works for any choice of x^1). If k=2, then, since $n\geq 5$, one easily check that X_1, \ldots, X_{2k} are disjoint by taking $x^1=\mathbf{0}$ and $x^3=\mathbf{1}$. Suppose now that $k\geq 3$ and choose $x^{2p-1}=e_{j_{2p-2}}$ for all $p\in [k]$, where j_0 means j_{2k} . Then each X_{2p-1} contains configurations of weight 1 or 3 and each X_{2p} contains configurations of weight 2. Hence, given $1\leq p< q\leq k$, we have to prove that $X_{2p-1}\cap X_{2q-1}=\emptyset$ and $X_{2p}\cap X_{2q}=\emptyset$. Suppose that $x\in X_{2p-1}\cap X_{2q-1}$. If w(x)=1 then we deduce that $x=e_{j_{2p-2}}=e_{j_{2q-2}}$ which is false since $p\neq q$. If w(x)=3 then $x_i=1$ for some $i\in I_{2p-1}$ while $y_i=0$ for all $y\in X_{2q-1}$, a contradiction. Thus $X_{2p-1}\cap X_{2q-1}=\emptyset$. Suppose now that $x\in X_{2p}\cap X_{2q}$. Then $x=e_{j_{2p-2}}+e_{i_{2p}}=e_{j_{2q-2}}+e_{i_{2q}}$ for some $i_{2p}\in I_{2p}$ and $i_{2q}\in I_{2q}$. Thus $i_{2p}=j_{2q-2}$ and $i_{2q}=j_{2p-2}$. Hence $j_{2q-2}\in I_{2p}$, and since p< q this implies q=p+1. Also, $j_{2p-1}\in I_{2q}$ and since p< q this implies p=1 and p=1, but then p=1 and p=1 since p=1 and p=1 since p=1 and p=1 and p=1 since p=1 since

C Lemma for the proof of Theorem 2

We prove Lemma 4, restated below. We first give some definitions. Given $X \subseteq \{0,1\}^n$ and $i \in [n]$, we say that X is closed by e_i if $X = X + e_i$. One easily check that if $X, Y \subseteq \{0,1\}^n$ are closed by e_i , then so is $X \cap Y$. Also, if |X| is closed by e_i then |X| is even. Indeed, let X_0 be the set of of $x \in X$ with $x_i = 0$ and $X_1 = X \setminus X_0$. We have $X_0 + e_i \subseteq X_1$, thus $|X_0| \le |X_1|$ and similarly, $X_1 + e_i \subseteq X_0$ thus $|X_1| \le |X_0|$. Hence $|X_0| = |X_1|$ so |X| is even.

Lemma 4. Let f be a n-component network and distinct $i, j \in [n]$. Some digraph in $\mathcal{G}(f)$ has no arc from j to i if and only if f has a (2^{n-2}) -nice set.

Proof. Let $h = \pi \circ f \circ \pi^{-1}$ for some permutation π of $\{0,1\}^n$, and suppose that G(h) has no arc from j to i. Let X be the set of $x \in \{0,1\}^n$ with $x_i = 0$, of size 2^{n-1} , and let $X^- = h^{-1}(X)$. If $x \in X^-$, that is, $h_i(x) = 0$, then $h_i(x + e_j) = 0$ since otherwise G(h) has an arc from j to i. Thus $x + e_j \in X^-$. Hence X^- is closed by e_j thus $|X^-|$ is even. Since $j \neq i$, X is also closed by e_j , so $X^- \cap X$ is closed by e_j and thus $|X^- \cap X|$ is even. Let $A = \pi^{-1}(X)$. Then one easily check that $f^{-1}(A) = \pi^{-1}(X^-)$ and that $f^{-1}(A) \cap A = \pi^{-1}(X^- \cap X)$. So $|f^{-1}(A)|$ and $|f^{-1}(A) \cap A|$ are even, and thus A is a (2^{n-2}) -nice set of f.

Conversely, suppose that f has a (2^{n-2}) -nice set A, thus of size 2^{n-1} . Let $A^- = f^{-1}(A)$. Then $|A|, |A^-|$ and $|A^- \cap A|$ are even, so $|A \setminus A^-|$ and $|A^- \setminus A|$ are also even. Hence there is a a balanced partition (A_1, A_2) of $A \cap A^-$, a balanced partition (A_3, A_4) of $A \setminus A^-$, and a balanced partition (A_3^-, A_4^-) of $A^- \setminus A$. Then (A_1, A_2, A_3, A_4) is a partition of A and (A_1, A_2, A_3^-, A_4^-) is a partition of A^- , and $A_1, A_2, A_3, A_4, A_3^-, A_4^-$ are disjoint.

For k=0,1, let Y_k be the set of $x\in\{0,1\}^n$ with $x_i=k$ and $x_j=0$. Since $|A|=2^{n-1}$ we have $|A_1|+|A_3|=2^{n-2}$ thus there is a partition (X_1,X_3) of Y_0 with $|X_1|=|A_1|$ and $|X_3|=|A_3|$. Since $|A_3^-|=|A^-\setminus A|/2\leq (2^n-|A|)/2=2^{n-2}$ there is $X_3^-\subseteq Y_1$ of size $|A_3^-|$. Let $X_2=X_1+e_j$, $X_4=X_3+e_j$ and $X_4^-=X_3^-+e_j$. Then $X_1,X_2,X_3,X_4,X_3^-,X_4^-$ are disjoint and of size $|A_1|,|A_2|,|A_3|,|A_4|,|A_3^-|,|A_4^-|$. Hence there is a permutation π of $\{0,1\}^n$ that sends $A_1,A_2,A_3,A_4,A_3^-,A_4^-$ on $X_1,X_2,X_3,X_4,X_3^-,X_4^-$, respectively.

Let $h = \pi \circ f \circ \pi^{-1}$. Let $X = X_1 \cup X_2 \cup X_3 \cup X_4$ and $X^- = X_1 \cup X_2 \cup X_3^- \cup X_4^-$. One easily check that: X is the set of $x \in \{0,1\}^n$ with $x_i = 0$; X^- is closed by e_j ; and $X^- = h^{-1}(X)$. We will prove that G(h) has no arc from j to i. Suppose, for a contradiction, that there is $x \in \{0,1\}^n$ with $h_i(x) \neq h_i(x + e_j)$. Without loss, we can assume that $h_i(x) = 0$, that is, $h(x) \in X$. So $x \in X^-$, hence $x + e_j \in X^-$, thus $h(x + e_j) \in X$, that is, $h_i(x + e_j) = 0$, a contradiction. Thus G(h) has no arc from j to i.

D Lemma for the proof of Theorem 3

For $X \subseteq \{0,1\}^n$, let $\partial(X)$ be the number of edges in Q_n with exactly one end in X; equivalently, it is the number of pairs (x,i) with $x \in X$ and $i \in [n]$ such that $x + e_i \notin X$. We can regard |X| as the volume of X and $\delta(X)$ as its perimeter and ask: what is the minimum perimeter for a given volume? The answer is Harp's isoperimetric inequality, from 1964 [2]. We denote by L_k the first k configurations in $\{0,1\}^n$ according to the lexicographic order (e.g. for n = 4 we have $L_5 = \{0000, 1000, 0100, 1100, 0010\}$).

Theorem 4 ([2]). If $n \ge 1$ and $X \subseteq \{0,1\}^n$ then $\partial(X) \ge \partial(L_{|X|})$.

In practice, the following approximation is often used; see [3] for instance.

Corollary 1. If $n \ge 1$ and $X \subseteq \{0,1\}^n$ is non-empty, then

$$\partial(X) \ge |X|(n - \log_2 |X|).$$

From this inequality, we deduce Lemma 7, that we restate.

Lemma 7. Let $A \subseteq \{0,1\}^n$ be non-empty, and let d be the average degree of the subgraph of Q_n induced by A. Then $|A| \ge 2^d$.

Proof. For $a \in A$, let d(a) be the degree of a in the subgraph of Q_n induced by A, and let d be the average degree, that is, $d = \sum_{a \in A} d(a)/|A|$. Since, for each $a \in A$, there are exactly n - d(a) components $i \in [n]$ such that $a + e_i \notin A$, we have, using Corollary 1,

$$\partial(A) = \sum_{a \in A} n - d(a) = |A|n - |A|d = |A|(n - d) \ge |A|(n - \log_2 |A|),$$

thus $d \leq \log_2 |A|$ as desired.